Journal of Combinatorial Theory, Series B 103 (2013) 21–45

Contents lists available at SciVerse ScienceDirect

Journal of Combinatorial Theory, Series B

www.elsevier.com/locate/jctb

Complex zero-free regions at large $|q|$ for multivariate Tutte polynomials (alias Potts-model partition functions) with general complex edge weights

Bill Jackson [a], Aldo Procacci [b], Alan D. Sokal [c,1]

[a] School of Mathematical Sciences, Queen Mary University of London, Mile End Road, London E1 4NS, United Kingdom
[b] Departamento de Matemática, Universidade Federal de Minas Gerais, Av. Antônio Carlos, 6627 – Caixa Postal 702, 30161-970 Belo Horizonte, MG, Brazil
[c] Department of Physics, New York University, 4 Washington Place, New York, NY 10003, USA

ARTICLE INFO

Article history:
Received 20 November 2009
Available online 15 September 2012

Keywords:
Graph
Chromatic polynomial
Multivariate Tutte polynomial
Potts model
Penrose identity
Penrose inequality
Lambert W function

ABSTRACT

We find zero-free regions in the complex plane at large $|q|$ for the multivariate Tutte polynomial (also known in statistical mechanics as the Potts-model partition function) $Z_G(q, \boldsymbol{w})$ of a graph G with general complex edge weights $\boldsymbol{w} = \{w_e\}$. This generalizes a result of Sokal (2001) [28] that applies only within the complex antiferromagnetic regime $|1 + w_e| \leqslant 1$. Our proof uses the polymer-gas representation of the multivariate Tutte polynomial together with the Penrose identity.

1. Introduction

A decade ago, Sokal [28] proved that if $G = (V, E)$ is a loopless graph[2] of maximum degree Δ, then all the roots (real or complex) of the chromatic polynomial $P_G(q)$ lie in the disc $|q| < C(\Delta)$, where $C(\Delta)$ are semi-explicit constants (given by a variational formula) satisfying $C(\Delta) \leqslant 7.963907\Delta$.[3] More

E-mail addresses: b.jackson@qmul.ac.uk (B. Jackson), aldo@mat.ufmg.br (A. Procacci), sokal@nyu.edu (A.D. Sokal).

1 Also at Department of Mathematics, University College London, London WC1E 6BT, England.

2 All graphs in this paper are finite and undirected; furthermore, they are *allowed* to contain loops and multiple edges unless we explicitly state otherwise.

3 More recently, Borgs [9] has provided a simpler variational characterization of the constant $K = \lim_{\Delta\to\infty} C(\Delta)/\Delta \approx 7.963906$ than the one given by Sokal [28, Proposition 5.4] – compare Eqs. (1.3a) and (1.3b) below – and Fernández and Procacci [14] have provided, in an analogous way, a simpler variational characterization of the constants $C(\Delta)$. Furthermore, Fernández and Procacci [14] have improved the constants $C(\Delta)$ to smaller constants $C^*(\Delta)$, for which $K^* = \lim_{\Delta\to\infty} C^*(\Delta)/\Delta \approx 6.907652$.

0095-8956/$ – see front matter
http://dx.doi.org/10.1016/j.jctb.2012.08.002

generally, Sokal proved a bound on the zeros of the multivariate Tutte polynomial (also known in statistical mechanics as the Potts-model partition function, see [30,26,34,35])

$$Z_G(q, \boldsymbol{w}) = \sum_{A \subseteq E} q^{k(A)} \prod_{e \in A} w_e \tag{1.1}$$

[here $k(A)$ denotes the number of connected components in the subgraph (V, A)] when the edge weights $\boldsymbol{w} = \{w_e\}$ lie in the "complex antiferromagnetic regime" $|1 + w_e| \leqslant 1$:

Theorem 1.1. *(See [28, Corollary 5.5].) Let $G = (V, E)$ be a loopless graph equipped with complex edge weights $\boldsymbol{w} = \{w_e\}_{e \in E}$ satisfying $|1 + w_e| \leqslant 1$ for all e. Then all the zeros of $Z_G(q, \boldsymbol{w})$ lie in the disc $|q| < K\Delta(G, \boldsymbol{w})$, where*

$$\Delta(G, \boldsymbol{w}) = \max_{x \in V} \sum_{e \ni x} |w_e| \tag{1.2}$$

and

$$K = \min\left\{L\colon \inf_{\alpha > 0} \alpha^{-1} \sum_{n=2}^{\infty} e^{\alpha n} L^{-(n-1)} \frac{n^{n-1}}{n!} \leqslant 1\right\} \tag{1.3a}$$

$$= \min_{a > 0} \frac{a + e^a}{\log(1 + a e^{-a})} \tag{1.3b}$$

$$\approx 7.963906075890002502\ldots. \tag{1.3c}$$

Moreover, we rigorously have $K \leqslant 7.963907$.

Here the simpler formula (1.3b) for the constant K is due to Borgs [9, Theorem 2.1].

The purpose of this paper is to extend Sokal's bound by removing the condition that $|1 + w_e| \leqslant 1$ for all e. More precisely, we shall prove[4]:

Theorem 1.2. *Let $G = (V, E)$ be a loopless graph equipped with complex edge weights $\boldsymbol{w} = \{w_e\}_{e \in E}$. Then all the zeros of $Z_G(q, \boldsymbol{w})$ lie in the disc*

$$|q| < \hat{\mathcal{K}}\big(\Psi(G, \boldsymbol{w})\big)\hat{\Delta}(G, \boldsymbol{w}), \tag{1.4}$$

where

$$\hat{\Delta}(G, \boldsymbol{w}) = \max_{x \in V} \sum_{\substack{e \ni x \\ e = xy}} \min\left\{|w_e|, \frac{|w_e|}{|1 + w_e|}\right\} \prod_{f \ni y} \max\{1, |1 + w_f|\}^{1/2}, \tag{1.5}$$

$$\Psi(G, \boldsymbol{w}) = \max_{x \in V} \prod_{e \ni x} \max\{1, |1 + w_e|\} \tag{1.6}$$

and

$$\hat{\mathcal{K}}(\psi) = \min\left\{L\colon \inf_{\alpha > 0} \big(e^{\alpha} - 1\big)^{-1} \sum_{n=2}^{\infty} e^{\alpha n} \psi^{1/2} L^{-(n-1)} \frac{n^{n-1}}{n!} \leqslant 1\right\} \tag{1.7a}$$

$$= \min_{1 < y < 1 + \psi^{-1/2}} \frac{\psi^{-1/2} y}{\big(1 + \psi^{-1/2} - y\big) \log y} \tag{1.7b}$$

[4] A simpler but weaker version of this result can be found in the first and second preprint versions of this paper (http://arxiv.org/abs/0810.4703v1 and v2).

$$= \psi^{-1/2} W\left(\frac{e}{1+\psi^{-1/2}}\right) \Big/ \left[1 - W\left(\frac{e}{1+\psi^{-1/2}}\right)\right]^2 \tag{1.7c}$$

$$\leqslant 4\psi^{1/2} + 3, \tag{1.7d}$$

where W is the Lambert W function [11], i.e. the inverse function to $x \mapsto xe^x$.

When $|1 + w_e| \leqslant 1$ for all e, we have $\hat{\Delta}(G, \boldsymbol{w}) = \Delta(G, \boldsymbol{w})$ and $\Psi(G, \boldsymbol{w}) = 1$, so that Theorem 1.2 reduces in this case to Theorem 1.1 with an improved constant [14] $K^* \equiv \hat{\mathcal{K}}(1) = W(e/2)/[1 - W(e/2)]^2 \approx 6.907651697774449218\ldots$. This explicit formula for the Fernández–Procacci [14] constant K^* appears to be new.

Let us also remark that the upper bound (1.7d) gives precisely the first two terms of the large-ψ asymptotics of $\hat{\mathcal{K}}(\psi)$: see Eq. (A.29) in Appendix A.

Please note that both $\Psi(G, \boldsymbol{w})$ and $\hat{\Delta}(G, \boldsymbol{w})$ involve a *product* over all edges incident to a given vertex rather than a sum, and hence grow *exponentially* (rather than linearly) with the vertex degree whenever $|1 + w_e| > 1$. The resulting exponential dependence of the bound on $|q|$ given in Theorem 1.2 is not merely an artifact of our proof, but is a genuine feature of the regime $|1 + w_e| > 1$.[5] To see this, it suffices to note that whenever one replaces an edge e by k edges in parallel, the effective couplings $w_{e,\mathrm{eff}} = (1 + w_e)^k - 1$ grow exponentially in k when $|1 + w_e| > 1$ but only linearly when $|1 + w_e| \leqslant 1$. For instance, the graph $G = K_2^{(k)}$ (a pair of vertices connected by k parallel edges) with all edge weights equal has $Z_G(q, w) = q[q + (1 + w)^k - 1]$, so that we must take $|q| > |(1 + w)^k - 1|$ to avoid a root. This has roughly (but not exactly) the same dependence in w and k as the bound of Theorem 1.2. See Example 7.3 below for details.

When all edge weights are equal, the two factors $\hat{\mathcal{K}}(\Psi(G, \boldsymbol{w}))$ and $\hat{\Delta}(G, \boldsymbol{w})$ combine to produce a bound that grows linearly with $\Psi(G, \boldsymbol{w})$ as $\Psi(G, \boldsymbol{w}) \to \infty$. If we restrict attention to *simple* graphs, then with a little more combinatorial work we can obtain a bound that grows only like $\Psi(G, \boldsymbol{w})^{1/2}$:

Theorem 1.3. *Let $G = (V, E)$ be a simple graph (i.e. no loops or multiple edges) equipped with complex edge weights $\boldsymbol{w} = \{w_e\}_{e\in E}$. Then all the zeros of $Z_G(q, \boldsymbol{w})$ lie in the disc*

$$|q| < K_\mu^* \Delta^*(G, \boldsymbol{w}), \tag{1.8}$$

where

$$\Delta^*(G, \boldsymbol{w}) = \max_{x\in V} \sum_{\substack{e\ni x\\ e=xy}} \min\left\{|w_e|, \frac{|w_e|}{|1 + w_e|^{1/2}}\right\} \prod_{f\ni y} \max\{1, |1 + w_f|\}^{1/2} \tag{1.9}$$

and $\mu = \hat{\Delta}(G, \boldsymbol{w})/\Delta^*(G, \boldsymbol{w})$ and

$$K_\mu^* = \min\left\{L:\ \inf_{\alpha>0} \left(e^\alpha - 1\right)^{-1} \sum_{n=2}^{\infty} e^{\alpha n} L^{-(n-1)} \frac{[1 + (n - 1)\mu]^{n-2}}{(n - 1)!} \leqslant 1\right\} \tag{1.10a}$$

$$= \min_{1<y<2} \frac{y^\mu}{(2 - y)\log y} \tag{1.10b}$$

$$\leqslant 5 + 2\mu. \tag{1.10c}$$

Please note that $0 < \mu \leqslant 1$ because $\min\{|w_e|, |w_e|/|1 + w_e|\} \leqslant \min\{|w_e|, |w_e|/|1 + w_e|^{1/2}\}$ for all $e \in E$, hence $\hat{\Delta}(G, \boldsymbol{w}) \leqslant \Delta^*(G, \boldsymbol{w})$. The constant K_μ^* is an increasing function of $\mu \in (0, 1]$, but the variation is fairly weak: we have $K_0^* = W(2e)/[2[W(2e) - 1]^2] \approx 4.892888$ and $K_1^* = K^* = W(e/2)/[1 - W(e/2)]^2 \approx 6.907652$. Thus, in the complex antiferromagnetic regime $|1 + w_e| \leqslant 1$ for all e, where $\mu = 1$, Theorems 1.2 and 1.3 give the same bound.

[5] See also [28, Remark 2 after Corollary 5.5].

When $|1+w_e|>1$, by contrast, Theorem 1.3 is in most cases a big improvement over Theorem 1.2: this is because K_μ^* is always order 1 while $\hat{\mathcal{K}}(\Psi(G,\boldsymbol{w}))$ is order $\Psi(G,\boldsymbol{w})^{1/2}$.

Note that the bound (1.4) involves a double maximum: once over $x \in V$ in $\Psi(G,\boldsymbol{w})$, and once over $x \in V$ in $\hat{\Delta}(G,\boldsymbol{w})$. Such a bound is "unnatural" in the sense that if G is a disjoint union $G = G_1 \uplus G_2$, then the chromatic roots of G are the union of those of G_1 and G_2, and $\hat{\mathcal{K}}(\Psi)$ and $\hat{\Delta}$ are each the maximum of those for G_1 and G_2, but the product $\hat{\mathcal{K}}(\Psi)\hat{\Delta}$ for G *can exceed* the maximum of those for G_1 and G_2 because one factor could be maximized for G_1 and the other for G_2 (see Example 7.7 below). The bound (1.8) has the virtue of avoiding such a double maximum. It is an open question whether a bound avoiding a double maximum can be obtained for non-simple graphs.

On the other hand, in the bound (1.8) we do pay a price, compared to (1.4), by having $\Delta^*(G,\boldsymbol{w})$ in place of $\hat{\Delta}(G,\boldsymbol{w})$, since as noted above we have $\Delta^*(G,\boldsymbol{w}) \geqslant \hat{\Delta}(G,\boldsymbol{w})$. In fact, the simple example $G = K_2$ shows that the bound of Theorem 1.3 can in some cases be inferior to that of Theorem 1.2, by a factor of up to $K_0^*/4 \approx 1.223222$ (see Examples 7.1 and 7.2 below). But this seems to be the largest possible ratio of the two bounds.

It is curious that the bound of Theorem 1.3 is not always better than that of Theorem 1.2, despite using better "ingredients" in its proof; the reasons for this will be discussed near the end of Section 6. It would be interesting to try to find a single natural bound that simultaneously improves Theorems 1.2 and 1.3.

Please note also (see e.g. [30]) that if G is a loopless graph with multiple edges, then its multivariate Tutte polynomial is identical to that of the underlying simple graph $\hat{G}$ in which each set of parallel edges $e_1,\ldots,e_k$ in G is replaced by a single edge e in $\hat{G}$ with weight $\hat{w}_e = \prod_{i=1}^k (1+w_{e_i}) - 1$. So one is always free to apply Theorem 1.2 or 1.3 to $(\hat{G},\hat{\boldsymbol{w}})$ instead of applying Theorem 1.2 to $(G,\boldsymbol{w})$. The following lemma concerning the behavior of $\Psi(G,\boldsymbol{w})$ and $\hat{\Delta}(G,\boldsymbol{w})$ under parallel reduction – which will be proven at the end of Section 6 – implies that the bound we get by applying Theorem 1.2 to $(\hat{G},\hat{\boldsymbol{w}})$ will never be worse than the bound we get by applying Theorem 1.2 to $(G,\boldsymbol{w})$. So we can find our best bound for any given (multi)graph G by constructing $(\hat{G},\hat{\boldsymbol{w}})$ and then taking the minimum of the bounds we obtain by applying (1.4) and (1.8) to $(\hat{G},\hat{\boldsymbol{w}})$.

Lemma 1.4. *Let $w_1, w_2 \in \mathbb{C}$ and put $w_3 = (1+w_1)(1+w_2) - 1$. Then*

$$\max\{1, |1+w_3|\} \leqslant \max\{1, |1+w_1|\} \max\{1, |1+w_2|\} \tag{1.11}$$

and

$$\min\left\{|w_3|, \frac{|w_3|}{|1+w_3|}\right\} \leqslant \min\left\{|w_1|, \frac{|w_1|}{|1+w_1|}\right\} + \min\left\{|w_2|, \frac{|w_2|}{|1+w_2|}\right\}. \tag{1.12}$$

Sokal's proof of Theorem 1.1 involved the following steps:

1. Write the multivariate Tutte polynomial $Z_G(q,\boldsymbol{w})$ as the partition function of a polymer gas with weights depending on q and $\boldsymbol{w}$ (this is easy: see Section 2 below).
2. Invoke the Kotecký–Preiss [21] condition for the nonvanishing of the partition function of a polymer gas.
3. Control the polymer weights by bounding sums over connected subgraphs by sums over trees, using the Penrose inequality [25]. This step required $|1+w_e| \leqslant 1$.
4. Bound the total weight of n-vertex trees (or more generally, of connected subgraphs with m edges) in G that contain a specified vertex $x \in V$.
5. Put everything together to prove that $Z_G(q,\boldsymbol{w}) \neq 0$ whenever q lies outside a specified disc.

Here we follow the same outline, but modify step 3 so as to allow arbitrary complex weights w_e. In addition, in step 2 we replace the Kotecký–Preiss condition by the more powerful Gruber–Kunz–Fernández–Procacci [16,13] condition, thereby slightly improving the numerical constant along the lines of the work of Fernández and Procacci [14] for chromatic polynomials. Finally, we need a slightly strengthened version of the bound in step 4.

The plan of this paper is to treat each of these five steps in successive sections. Thus, in Section 2 we recall how the multivariate Tutte polynomial $Z_G(q, \boldsymbol{w})$ can be written as the partition function of a polymer gas. In Section 3 we recall the Kotecký–Preiss and Gruber–Kunz–Fernández–Procacci conditions for the nonvanishing of the partition function of a polymer gas. In Section 4 we recall the Penrose identity [25] and show how to use it to bound the polymer weights *without* assuming that $|1 + w_e| \leqslant 1$; this is our main new contribution. In Section 5 we prove a bound on the total weight of connected m-edge subgraphs in G that contain a specified vertex x; this strengthens the bound of [28,17] by taking specific account of the edges incident on x and by introducing vertex weights. In Section 6 we put everything together to prove Theorems 1.2 and 1.3; we also prove Lemma 1.4. Finally, in Section 7 we examine some examples that shed light on the extent to which Theorems 1.2 and 1.3 are sharp or non-sharp. In Appendix A we prove Lemma 6.1 and some related facts.

2. Polymer-gas representation of $Z_G(q, w)$

In statistical mechanics, an *abstract polymer gas* is a triple $(P, \xi, \mathcal{R})$ where P is a finite set (whose elements are called "polymers"), ξ is a complex-valued function defined on P (the value $\xi(p)$ is called the "activity" or "fugacity" or "weight" of the polymer $p \in P$), and $\mathcal{R} \subseteq P \times P$ is a symmetric and reflexive relation (called the "incompatibility relation"). Note that, since $\mathcal{R}$ is supposed reflexive, we have $(p, p) \in \mathcal{R}$ for all $p \in P$. Then the *partition function* of the polymer gas $(P, \xi, \mathcal{R})$ – a key quantity from which all thermodynamic properties of the system can in principle be derived – is defined by

$$\Xi(\xi) = \sum_{n=0}^{\infty} \sum_{\substack{\{p_1,\ldots,p_n\} \subseteq P \\ (p_i,p_j) \notin \mathcal{R} \ \forall i \neq j}} \xi(p_1) \cdots \xi(p_n) \tag{2.1}$$

where the sum runs over unordered collections $\{p_1, \ldots, p_n\}$ of mutually compatible elements of P, and the $n = 0$ term in the sum is understood to contribute 1.

In this section we recall how to rewrite the multivariate Tutte polynomial $Z_G(q, \boldsymbol{w})$ of a graph $G = (V, E)$ as the partition function of a polymer gas living on the vertex set of G, i.e. an abstract polymer gas whose polymers are nonempty subsets of V. This easy result is due to Sokal and Kupiainen [28, Proposition 2.1].

First, some notation: If $H = (\mathsf{V}, \mathsf{E})$ is a graph equipped with edge weights $\boldsymbol{w} = \{w_e\}_{e \in \mathsf{E}}$, we denote by $C_H(\boldsymbol{w})$ the generating polynomial of connected spanning subgraphs of H, i.e.

$$C_H(\boldsymbol{w}) = \sum_{\substack{A \subseteq \mathsf{E} \\ (\mathsf{V}, A) \text{ connected}}} \prod_{e \in A} w_e. \tag{2.2}$$

Note that $C_H(\boldsymbol{w}) \equiv 0$ if H is disconnected.

If $G = (V, E)$ is a graph and $S \subseteq V$, we denote by $G[S]$ the induced subgraph of G on S, i.e. $G[S]$ is the graph whose vertex set is S and whose edges consist of all the edges of G both of whose endpoints lie in S.

Proposition 2.1 *(Polymer representation of the multivariate Tutte polynomial). Let $G = (V, E)$ be a loopless graph equipped with edge weights $\boldsymbol{w} = \{w_e\}_{e \in E}$. Then*

$$q^{-|V|} Z_G(q, \boldsymbol{w}) = \sum_{N=0}^{\infty} \sum_{\substack{\{S_1,\ldots,S_N\} \\ \text{disjoint}}} \prod_{i=1}^{n} \xi(S_i), \tag{2.3}$$

where the sum runs over unordered collections $\{S_1, \ldots, S_N\}$ of disjoint nonempty subsets of V, and the weights $\xi(S)$ are given by

$$\xi(S) = \begin{cases} q^{-(|S|-1)} C_{G[S]}(\boldsymbol{w}) & \text{if } |S| \geqslant 2, \\ 0 & \text{if } |S| = 1. \end{cases} \tag{2.4}$$

[*The* $N = 0$ *term in the sum* (2.3) *is understood to contribute* 1.]

The identity (2.3) thus represents $q^{-|V|} Z_G(q, \boldsymbol{w})$ as the partition function of a polymer gas given by the triple $(P, \xi, \mathcal{R})$ with the polymer space P being the set of all nonempty subsets of V, the activity ξ being the function defined in (2.4), and the incompatibility relation $\mathcal{R}$ being nonempty intersection, i.e. $(S, S') \in \mathcal{R}$ if and only if $S \cap S' \neq \varnothing$. Note that, since the weight $\xi(S)$ vanishes for sets of cardinality 1 and also vanishes whenever the induced subgraph $G[S]$ is disconnected, we can equivalently restrict our polymer set P to be the set of all subsets $S \subseteq V$ of cardinality at least 2 and for which $G[S]$ is connected.

Hereafter we will refer to a polymer gas in which polymers are subsets of a given set V and the incompatibility relation is nonempty intersection as "a gas of nonoverlapping polymers living on V".

Proof of Proposition 2.1. Starting from the definition (1.1) of $Z_G(q, \boldsymbol{w})$, let us separate the terms in the sum according to the number k of connected components [i.e. $k(A) = k$] and according to the partition $\{S_1, \ldots, S_k\}$ of V that is induced by the vertex sets of those connected components; we will then sum over all ways of choosing edges within those vertex sets S_i so as to connect those vertices. We thus have

$$Z_G(q, \boldsymbol{w}) = q^{|V|} \sum_{k \geqslant 1} \sum_{\substack{\{S_1, \ldots, S_k\} \\ V = \biguplus S_i}} \prod_{i=1}^{k} q^{-(|S_i|-1)} C_{G[S_i]}(\boldsymbol{w}), \tag{2.5}$$

where the sum runs over all unordered partitions $\{S_1, \ldots, S_k\}$ of V into nonempty subsets, and we have used $|V| = \sum_{i=1}^{k} |S_i|$. Note now that any set S_i of cardinality 1 gets weight $q^{-(|S_i|-1)} C_{G[S_i]}(\boldsymbol{w}) = 1$ (here we have used the fact that G is loopless). So let us define $\{S'_1, \ldots, S'_N\}$ to be the subcollection of $\{S_1, \ldots, S_k\}$ consisting of the sets of cardinality $\geqslant 2$; and let us note that there is a one-to-one correspondence between unordered partitions $\{S_1, \ldots, S_k\}$ of V into nonempty subsets and unordered collections $\{S'_1, \ldots, S'_N\}$ of disjoint subsets of V of cardinality at least 2 (which need not cover all of V: indeed, the points not covered correspond to the singleton sets S_i in the original partition). Passing to $\{S'_1, \ldots, S'_N\}$ and dropping the primes, we have (2.3)/(2.4). □

3. Sufficient condition for the nonvanishing of a polymer-gas partition function

Let V be a finite set, and let $\{\rho(S)\}_{\varnothing \neq S \subseteq V}$ be a collection of complex weights associated to the nonempty subsets of V. Consider now a gas of nonoverlapping polymers living on V, with weights $\rho(S)$: the partition function of such a polymer gas is, by definition,

$$\Xi = \sum_{N=0}^{\infty} \sum_{\substack{\{S_1, \ldots, S_N\} \\ \text{disjoint}}} \prod_{i=1}^{N} \rho(S_i), \tag{3.1}$$

where the sum runs over unordered collections $\{S_1, \ldots, S_N\}$ of disjoint nonempty subsets of V, and the $N = 0$ term in (3.1) is understood to contribute 1. The following proposition – essentially proven almost four decades ago by Gruber and Kunz [16, Section 4, cf. Eq. (33)] but largely forgotten, and then rediscovered very recently by Fernández and Procacci [13, Eq. (3.17)] with a new proof – gives a sufficient condition for the nonvanishing of a polymer-gas partition function:

Proposition 3.1 *(Gruber–Kunz–Fernández–Procacci condition). Let V be a finite set, and let $\{\rho(S)\}_{\varnothing \neq S \subseteq V}$ be complex weights associated to the nonempty subsets of V. Suppose that there exists a number $\alpha > 0$ such that*

$$\sup_{x \in V} \sum_{S \ni x} e^{\alpha |S|} |\rho(S)| \leqslant e^{\alpha} - 1. \tag{3.2}$$

Then

$$\Xi \equiv \sum_{N=0}^{\infty} \sum_{\substack{\{S_1,\ldots,S_N\} \\ \text{disjoint}}} \prod_{i=1}^{n} \rho(S_i) \neq 0. \tag{3.3}$$

See also [6] for an extremely simple proof of Proposition 3.1 by induction on V.

In the slightly less powerful Kotecký–Preiss [21] condition, the term $e^\alpha - 1$ on the right-hand side of (3.2) is replaced by α.

Remark. Suppose that (as happens in all nontrivial cases) there exists a set S with $|S| \geqslant 2$ and $\rho(S) \neq 0$. Then the hypothesis that there exists $\alpha > 0$ such that (3.2) holds can be rewritten as

$$\inf_{\alpha>0} \bigl(e^\alpha - 1\bigr)^{-1} \sup_{x\in V} \sum_{S \ni x} e^{\alpha|S|} \bigl|\rho(S)\bigr| \leqslant 1, \tag{3.4}$$

since in this case the infimum on the left-hand side of (3.4) will always be attained at some $\alpha > 0$.[6] We will use the Gruber–Kunz–Fernández–Procacci condition in the form (3.4).

4. A bound on $C_H(\boldsymbol{w})$ via the Penrose identity

In this section we recall the Penrose identity [25] and show how it can be used to bound a sum over connected subgraphs by a sum over trees *even in the absence of the hypothesis* $|1 + w_e| \leqslant 1$.

Let $H = (\mathsf{V}, \mathsf{E})$ be a graph. Recall that $C_H(\boldsymbol{w})$ denotes the generating polynomial of connected spanning subgraphs of H:

$$C_H(\boldsymbol{w}) = \sum_{\substack{A\subseteq \mathsf{E} \\ (\mathsf{V},A)\ \text{connected}}} \prod_{e\in A} w_e. \tag{4.1}$$

We denote by $T_H(\boldsymbol{w})$ the generating polynomial of spanning trees in H:

$$T_H(\boldsymbol{w}) = \sum_{\substack{A\subseteq \mathsf{E} \\ (\mathsf{V},A)\ \text{tree}}} \prod_{e\in A} w_e. \tag{4.2}$$

Let $\mathcal{C}$ (resp. $\mathcal{T}$) be the set of subsets $A \subseteq \mathsf{E}$ such that (V, A) is connected (resp. is a tree). Clearly $\mathcal{C}$ is an increasing family of subsets of E with respect to set-theoretic inclusion, and the minimal elements of $\mathcal{C}$ are precisely those of $\mathcal{T}$ (i.e. the spanning trees). It is a nontrivial combinatorial fact – apparently first discovered by Penrose [25] – that the (anti-)complex $\mathcal{C}$ is *partitionable*: that is, there exists a map $\mathbf{R} : \mathcal{T} \to \mathcal{C}$ such that $\mathbf{R}(T) \supseteq T$ for all $T \in \mathcal{T}$ and $\mathcal{C} = \biguplus_{T\in\mathcal{T}} [T, \mathbf{R}(T)]$ (disjoint union), where $[E_1, E_2]$ denotes the Boolean interval $\{A\colon\ E_1 \subseteq A \subseteq E_2\}$. We call any such map $\mathbf{R}$ a *partition scheme*. In fact, many alternative choices of $\mathbf{R}$ are available,[7] and most of our arguments will not depend on any specific choice of $\mathbf{R}$. An immediate consequence of the existence of $\mathbf{R}$ is the following simple but fundamental identity:

---

[6] If there exists a set S with $|S| \geqslant 2$ and $\rho(S) \neq 0$, then the function $f(\alpha)$ being minimized on the left-hand side of (3.4) is a continuous function that tends to $+\infty$ as $\alpha \downarrow 0$ and as $\alpha \uparrow \infty$, hence its minimum is attained.

There is one exceptional case in which (3.4) holds but there does not exist $\alpha > 0$ such that (3.2) holds: namely, if $\rho(S) = 0$ whenever $|S| \geqslant 2$ and in addition we have $\max_{x\in V} |\rho(\{x\})| = 1$. Indeed, if $\rho(S) = 0$ for $|S| \geqslant 2$, we have $\Xi = \prod_{x\in V} [1 + \rho(\{x\})]$, which vanishes when at least one $\rho(\{x\})$ equals -1; so (3.4) *fails* (barely) to imply $\Xi \neq 0$ in this case.

[7] See for example [25], [7, Sections 7.2 and 7.3], [37, Section 8.3], [15, Sections 2 and 6], [5, Proposition 13.7 et seq.], [28, Proposition 4.1] and [27, Lemma 2.2].

Proposition 4.1 *(Penrose identity). (See [25].) Let* $\mathbf{R} : \mathcal{T} \to \mathcal{C}$ *be any partition scheme. Then*

$$C_H(\boldsymbol{w}) = \sum_{\substack{T \subseteq \mathsf{E} \\ (\mathsf{V},T)\ \text{tree}}} \prod_{e \in T} w_e \sum_{T \subseteq A \subseteq \mathbf{R}(T)} \prod_{e \in A \setminus T} w_e \tag{4.3a}$$

$$= \sum_{\substack{T \subseteq \mathsf{E} \\ (\mathsf{V},T)\ \text{tree}}} \prod_{e \in T} w_e \prod_{e \in \mathbf{R}(T) \setminus T} (1 + w_e). \tag{4.3b}$$

If $|1 + w_e| \leqslant 1$ for all e, then it is obvious that we can take absolute values everywhere in (4.3b) and drop the factors $|1 + w_e|$, yielding:

Proposition 4.2 *(Penrose inequality). (See [25].) Let* $H = (\mathsf{V}, \mathsf{E})$ *be a graph equipped with complex edge weights* $\boldsymbol{w} = \{w_e\}_{e \in \mathsf{E}}$ *satisfying* $|1 + w_e| \leqslant 1$ *for all* e*. Then*

$$\bigl|C_H(\boldsymbol{w})\bigr| \leqslant T_H\bigl(|\boldsymbol{w}|\bigr). \tag{4.4}$$

Remark. By using a specific choice of the map $\mathbf{R}$ (namely, that of Penrose [25]), Fernández and Procacci [13] have recently shown how to improve Proposition 4.2 when $w_e \in \{-1, 0\}$ for all e; and this improvement plays a key role in their proof of the Gruber–Kunz–Fernández–Procacci condition (Proposition 3.1) for polymer gases with hard-core repulsive interactions. See also Fernández et al. [12] for a generalization to $-1 \leqslant w_e \leqslant 0$, which leads to an improved convergence criterion for the Mayer expansion in lattice gases with soft repulsive interactions.

Let us now show what can be done *without* the hypothesis $|1 + w_e| \leqslant 1$. Given a vertex x in a graph $H = (\mathsf{V}, \mathsf{E})$, we denote by $\mathsf{E}(x)$ the set of edges of H incident on x. For any subset $A \subseteq \mathsf{E}$, let us write

$$A_+ = \bigl\{e \in A\colon\ |1 + w_e| > 1\bigr\}, \tag{4.5a}$$

$$A_- = \bigl\{e \in A\colon\ |1 + w_e| \leqslant 1\bigr\}. \tag{4.5b}$$

Proposition 4.3 *(Extended Penrose inequality). Let* $H = (\mathsf{V}, \mathsf{E})$ *be a loopless graph equipped with complex edge weights* $\boldsymbol{w} = \{w_e\}_{e \in \mathsf{E}}$*. Then*

$$\bigl|C_H(\boldsymbol{w})\bigr| \leqslant T_H\bigl(\bigl|\boldsymbol{w}'\bigr|\bigr) \prod_{e \in \mathsf{E}} \max\bigl\{1, |1 + w_e|\bigr\} \tag{4.6a}$$

$$= T_H\bigl(\bigl|\boldsymbol{w}'\bigr|\bigr) \prod_{y \in \mathsf{V}} \prod_{e \in \mathsf{E}(y)} \max\bigl\{1, |1 + w_e|\bigr\}^{1/2} \tag{4.6b}$$

where

$$w'_e = \begin{cases} w_e & \text{if } |1 + w_e| \leqslant 1, \\ \frac{w_e}{1 + w_e} & \text{if } |1 + w_e| > 1. \end{cases} \tag{4.7}$$

Note that if $|1 + w_e| \leqslant 1$ for all e, then $\boldsymbol{w}' = \boldsymbol{w}$ and $\max\{1, |1 + w_e|\} = 1$ for all e, so Proposition 4.3 is a genuine extension of Proposition 4.2.

Proof of Proposition 4.3. In the Penrose identity (4.3b), multiply and divide the summand by $\prod_{e \in T_+}(1 + w_e)$: this yields

$$C_H(\boldsymbol{w}) = \sum_{\substack{T \subseteq \mathsf{E} \\ (\mathsf{V},T)\ \text{tree}}} \prod_{e \in T} w'_e \prod_{e \in (\mathbf{R}(T) \setminus T) \cup T_+} (1 + w_e). \tag{4.8}$$

Taking absolute values and using the trivial bound

$$\prod_{e \in (\mathbf{R}(T) \setminus T) \cup T_+} |1 + w_e| \leqslant \prod_{e \in \mathsf{E}} \max\{1, |1 + w_e|\}, \tag{4.9}$$

we obtain (4.6a). Then (4.6b) follows by observing that each edge $e \in \mathsf{E}$ is incident on precisely two vertices (since H is loopless). □

Remark. Quite a lot has been thrown away in (4.9). Can we do better in a usable way?

If we assume that the graph H is *simple* (i.e. has no loops or multiple edges), then we can get a slightly better bound:

Proposition 4.4 *(Extended Penrose inequality for simple graphs). Let $H = (\mathsf{V}, \mathsf{E})$ be a* simple *graph (i.e. no loops or multiple edges) equipped with complex edge weights $\boldsymbol{w} = \{w_e\}_{e \in \mathsf{E}}$. Then, for any vertex $x \in \mathsf{V}$, we have*

$$\bigl|C_H(\boldsymbol{w})\bigr| \leqslant T_H\bigl(\bigl|\boldsymbol{w}^{[x]}\bigr|\bigr) \prod_{e \in \mathsf{E} \setminus \mathsf{E}(x)} \max\{1, |1 + w_e|\} \tag{4.10a}$$

$$\leqslant T_H\bigl(\bigl|\tilde{\boldsymbol{w}}^{[x]}\bigr|\bigr) \prod_{y \in V \setminus \{x\}} \prod_{e \in \mathsf{E}(y)} \max\{1, |1 + w_e|\}^{1/2} \tag{4.10b}$$

where

$$w_e^{[x]} = \begin{cases} w_e & \text{if } |1 + w_e| \leqslant 1 \text{ or } e \in \mathsf{E}(x), \\ \frac{w_e}{1 + w_e} & \text{if } |1 + w_e| > 1 \text{ and } e \in \mathsf{E} \setminus \mathsf{E}(x) \end{cases} \tag{4.11}$$

and

$$\tilde{w}_e^{[x]} = \begin{cases} w_e & \text{if } |1 + w_e| \leqslant 1, \\ \frac{w_e}{|1 + w_e|^{1/2}} & \text{if } |1 + w_e| > 1 \text{ and } e \in \mathsf{E}(x), \\ \frac{w_e}{|1 + w_e|} & \text{if } |1 + w_e| > 1 \text{ and } e \in \mathsf{E} \setminus \mathsf{E}(x). \end{cases} \tag{4.12}$$

Please note that (4.10b) is indeed an improvement of (4.6b), because the product $\prod_{e \in \mathsf{E}(x)} \max\{1, |1 + w_e|\}^{1/2}$ more than compensates the factors $|\tilde{w}_e^{[x]}/w'_e| = \max\{1, |1 + w_e|\}^{1/2}$ for the *subset* of edges in $\mathsf{E}(x)$ that happen to lie in any given spanning tree T.

The proof of Proposition 4.4 will be based on the following key combinatorial fact (to be proven later):

Lemma 4.5. *Let $H = (\mathsf{V}, \mathsf{E})$ be a* simple *graph and let $x \in \mathsf{V}$ be any vertex. Then there exists a partition scheme $\mathbf{R}$ with the property that $\mathbf{R}(T) \setminus T$ does not contain any edge incident on x.*

Proof of Proposition 4.4, assuming Lemma 4.5. In the Penrose identity (4.3b), multiply and divide the summand by $\prod_{e \in [T \setminus \mathsf{E}(x)]_+} (1 + w_e)$: this yields

$$C_H(\boldsymbol{w}) = \sum_{\substack{T \subseteq \mathsf{E} \\ (\mathsf{V}, T) \text{ tree}}} \prod_{e \in T} w_e^{[x]} \prod_{e \in [\mathbf{R}(T) \setminus T] \cup [T \setminus \mathsf{E}(x)]_+} (1 + w_e). \tag{4.13}$$

Choosing the partition scheme as in Lemma 4.5, we have $\mathbf{R}(T) \setminus T \subseteq \mathsf{E} \setminus \mathsf{E}(x)$ and hence

$$\prod_{e \in [\mathbf{R}(T) \setminus T] \cup [T \setminus \mathsf{E}(x)]_+} |1 + w_e| \leqslant \prod_{e \in \mathsf{E} \setminus \mathsf{E}(x)} \max\{1, |1 + w_e|\}. \tag{4.14}$$

Taking absolute values in (4.13) and using (4.14), we obtain

$$\left|C_H(\boldsymbol{w})\right| \leqslant \sum_{\substack{T\subseteq \mathsf{E} \\ (\mathsf{V},T)\text{ tree}}} \prod_{e\in T}\left|w_e^{[x]}\right| \prod_{e\in \mathsf{E}\setminus \mathsf{E}(x)} \max\bigl\{1,|1+w_e|\bigr\}, \tag{4.15}$$

which is (4.10a).

Now observe that

$$\prod_{e\in \mathsf{E}\setminus \mathsf{E}(x)} \max\bigl\{1,|1+w_e|\bigr\} = \frac{\prod_{y\in V\setminus x}\prod_{e\in \mathsf{E}(y)}\max\{1,|1+w_e|\}^{1/2}}{\prod_{e\in \mathsf{E}(x)}\max\{1,|1+w_e|\}^{1/2}} \tag{4.16}$$

since the numerator of (4.16) counts every edge in $\mathsf{E}\setminus \mathsf{E}(x)$ twice and every edge in $\mathsf{E}(x)$ once. If in the denominator of (4.16) we replace the product over $e\in \mathsf{E}(x)$ by the smaller product over $e\in \mathsf{E}(x)\cap T$, we get an upper bound; inserting this into (4.15) yields (4.10b). □

Let us conclude this section by proving Lemma 4.5. This proof – unlike all the preceding results in this section – depends on a specific choice of the map $\mathbf{R}$, namely the one used by Penrose in his original paper [25]. Let us briefly recall Penrose's construction (see [13,12] for more details). We assume that $H=(\mathsf{V},\mathsf{E})$ is a *simple* graph, and we choose (arbitrarily) an ordering of the vertex set V by numbering the vertices $1,2,\ldots,n$ (where $n=|\mathsf{V}|$). We consider the vertex 1 to be the root, and denote it by r. If $T\subseteq \mathsf{E}$ is the edge set of a spanning tree in H [that is, (V,T) is a tree], then for each $x\in \mathsf{V}$ we denote by $\mathrm{dist}_T(x)$ the graph-theoretic distance in the tree (V,T) from the root r to the vertex x. Given T, the vertex set V is thus partitioned into "generations", defined as the sets of vertices at a given distance from the root r.

The Penrose map $\mathbf{R}: T\mapsto \mathbf{R}(T)$ is then defined as follows. For any tree $T\subseteq \mathsf{E}$, the edge set $\mathbf{R}(T)\supseteq T$ is obtained from T by adjoining all edges $e\in \mathsf{E}$ that either

(a) connect two vertices in the same generation [i.e. at equal distance from the root r in the tree (V,T) – note that no such edge can belong to T], or
(b) connect a vertex x to a vertex x' in the preceding generation [i.e. with $\mathrm{dist}_T(x')=\mathrm{dist}_T(x)-1$] that is higher-numbered than the parent of x [here the parent of x is the unique vertex y with $\mathrm{dist}_T(y)=\mathrm{dist}_T(x)-1$ such that $xy\in T$].

It can be shown [25,13,12] that $\mathbf{R}$ is indeed a partitioning map in the sense that $\mathcal{C}$ is the disjoint union of Boolean intervals $[T,\mathbf{R}(T)]$. Furthermore, it follows immediately from this construction that $\mathbf{R}(T)\setminus T$ cannot contain any edge incident on the root r; that is, $\mathbf{R}(T)\setminus T\subseteq \mathsf{E}\setminus \mathsf{E}(r)$.[8] Since any vertex could have been chosen as the root, Lemma 4.5 is proven.

Remark. Lemma 4.5 suggests the following combinatorial question: Let $H=(\mathsf{V},\mathsf{E})$ be a graph (simple or not). For which subsets $S\subseteq \mathsf{E}$ does there exist a partition scheme $\mathbf{R}$ with the property that $\mathbf{R}(T)\setminus T\subseteq \mathsf{E}\setminus S$ for all T? The same question can also be posed for matroids.

---

[8] We remark that this would no longer be the case in a generalization to the Penrose construction to non-simple graphs. In such a generalization, we would also order the edges connecting each pair of vertices, and we would add to the definition of $\mathbf{R}(T)$ a third case:

(c) connect a vertex x to its parent y by any edge that is higher-numbered than the edge connecting x to y in T.

We would then no longer be able to guarantee that $\mathbf{R}(T)\setminus T$ contains no edges incident on the root r; rather, we could assert only that $\mathbf{R}(T)\setminus T$ cannot contain any edge incident on the root r that is the *lowest-numbered* among its set of parallel edges.

5. Bounds on connected m-edge subgraphs containing a specified vertex

In this section consider a loopless graph $G = (V, E)$ equipped with nonnegative real edge weights $\{w_e\}_{e\in E}$ *and* nonnegative real vertex weights $\{w_v\}_{v\in V}$. Let us define the weighted sum over connected subgraphs $G' = (V', E') \subseteq G$ that contain a specified vertex x and have exactly m edges:

$$c_m(x; G, \boldsymbol{w}) = \sum_{\substack{G'=(V',E')\subseteq G \\ G' \text{ connected} \\ V'\ni x \\ |E'|=m}} \prod_{e\in E'} w_e \prod_{v\in V'} w_v, \tag{5.1}$$

where we write $\boldsymbol{w} = \{w_e\}_{e\in E} \cup \{w_v\}_{v\in V}$. We will abbreviate $c_m(x; G, \boldsymbol{w})$ to $c_m(x)$ when it is obvious which weighted graph $(G, \boldsymbol{w})$ we are referring to. Now define the weighted degree at x by

$$d(x; G, \boldsymbol{w}) = \sum_{e=xy\in E} w_e w_y \tag{5.2}$$

(note that this contains a factor w_y for each edge $e = xy$ incident to x but *not* a factor w_x), and define the maximum weighted degree by

$$\Delta(G, \boldsymbol{w}) = \max_{x\in V} d(x; G, \boldsymbol{w}). \tag{5.3}$$

The following bound on $c_m(x)$ extends an earlier result of the third author [28, Proposition 4.5], which is obtained by putting $w_v = 1$ for all $v \in V$ and using the fact that both $d(x; G, \boldsymbol{w})$ and $\Delta(G - x, \boldsymbol{w}|_{G-x})$ are bounded above by $\Delta(G, \boldsymbol{w})$.

Proposition 5.1. *Let $G = (V, E)$ be a loopless graph equipped with nonnegative real weights $\boldsymbol{w} = \{w_e\}_{e\in E} \cup \{w_v\}_{v\in V}$, and let $x \in V$. Suppose that either $w_v \geqslant 1$ for all $v \in V$ or G is simple. Then*

$$c_m(x) \leqslant \frac{w_x d(x; G, \boldsymbol{w})[d(x; G, \boldsymbol{w}) + m\Delta(G - x, \boldsymbol{w}|_{G-x})]^{m-1}}{m!} \tag{5.4}$$

for all $m \geqslant 0$.

We remark that the bound (5.4) need not hold if we remove the hypothesis that either $w_v \geqslant 1$ for all $v \in V$ or G is simple. Consider, for instance, the graph $G = K_2^{(m)}$ consisting of two vertices x, y joined by $m \geqslant 2$ parallel edges. Put $w_x = w_y = w$ and $w_e = 1$ for all $e \in E$. Then $c_m(x) = w^2$, while the right-hand side of (5.4) is $m^m w^{m+1}/m!$, which is less than $c_m(x)$ when w is small enough.

In the proof of Proposition 5.1 it will be convenient to employ the quantities

$$C(m, \kappa) = \begin{cases} \kappa(m+\kappa)^{m-1}/m! & \text{for } m \geqslant 1, \\ 1 & \text{for } m = 0 \end{cases} \tag{5.5}$$

defined for integer $m \geqslant 0$ and real κ. Then (5.4) can be rewritten in the form

$$c_m(x) \leqslant w_x C(m, d/\Delta)\Delta^m \tag{5.6}$$

where $d = d(x; G, \boldsymbol{w})$ and $\Delta = \Delta(G - x, \boldsymbol{w}|_{G-x})$.

Our proof of Proposition 5.1 uses induction on m, and is similar to the first proof of [17, Proposition 7.1]. It relies on the following properties of $C(m, \kappa)$:

(a) For each integer $m \geqslant 0$, $C(m, \kappa)$ is a polynomial of degree m in κ, with nonnegative coefficients. In particular, $C(m, \kappa)$ is an increasing function of κ for real $\kappa \geqslant 0$.
(b) Generating function: If $\mathsf{C}(z)$ solves the equation

$$\mathsf{C}(z) = e^{z\mathsf{C}(z)}, \tag{5.7}$$

then

$$\mathsf{C}(z)^\kappa = \sum_{m=0}^{\infty} C(m,\kappa) z^m \tag{5.8}$$

for all real κ; this follows from the Lagrange inversion formula. Moreover, the series (5.8) is absolutely convergent for $|z| \leqslant 1/e$ and satisfies $\mathsf{C}(1/e) = e$.

(c) For integer $k \geqslant 1$,

$$C(m,k) = \sum_{\substack{m_1,\dots,m_k \geqslant 0\\ m_1+\dots+m_k=m}} \prod_{i=1}^{k} C(m_i,1). \tag{5.9}$$

This is an immediate consequence of (5.8).

(d) For all real κ and z,

$$C(m,\kappa) = \sum_{f=0}^{m} \frac{z^f}{f!} C(m-f, \kappa - z + f). \tag{5.10}$$

See [17, Eq. (7.7)].

For any subset $F \subseteq E$, we use the notation $w(F) = \prod_{e\in F} w_e$. Also, for any $F \subseteq E(x)$, we denote by Y^F the set of vertices of $V - x$ that are incident with edges in F, and we write $j(F) = |Y^F|$ for the number of such vertices. Please observe that $j(F) \leqslant |F|$; and if the graph G is simple, then $j(F) = |F|$.

Our proof of Proposition 5.1 will be based on the following two lemmas:

Lemma 5.2. *Let $G = (V, E)$ be a loopless graph equipped with nonnegative real weights $\boldsymbol{w} = \{w_e\}_{e\in E} \cup \{w_v\}_{v\in V}$, and let $x \in V$. For each $F \subseteq E(x)$, let $Y^F = \{x_1^F, x_2^F, \dots, x_{j(F)}^F\}$ be a labeling of the vertices of $V - x$ that are incident with edges in F. Then, for all $m \geqslant 1$,*

$$c_m(x; G, \boldsymbol{w}) \leqslant w_x \sum_{\varnothing \neq F \subseteq E(x)} w(F) \sum_{\substack{m_1,\dots,m_{j(F)} \geqslant 0\\ m_1+\dots+m_{j(F)}=m-|F|}} \prod_{i=1}^{j(F)} c_{m_i}\left(x_i^F; G-x, \boldsymbol{w}|_{G-x}\right). \tag{5.11}$$

Proof. Similar to that given for Facts 1 and 2 in [17, Section 7]. $\square$

Lemma 5.3. *(See [17, Lemma 7.2].) Let S be a set in which each element $e \in S$ is given a nonnegative real weight w_e. Then, for each integer $f \geqslant 0$, we have*

$$\sum_{\substack{F\subseteq S\\ |F|=f}} w(F) \leqslant \frac{1}{f!}\left(\sum_{e\in S} w_e\right)^f. \tag{5.12}$$

Proof of Proposition 5.1. Let $d = d(x; G, \boldsymbol{w})$ and $\Delta = \Delta(G - x, \boldsymbol{w}|_{G-x})$. We will prove (5.4)/(5.6) by induction on m. The statement holds trivially when $m = 0$, so let us assume that $m \geqslant 1$. By Lemma 5.2,

$$\begin{aligned} c_m(x) &\leqslant w_x \sum_{\varnothing \neq F \subseteq E(x)} w(F) \sum_{\substack{m_1,\dots,m_{j(F)} \geqslant 0\\ m_1+\dots+m_{j(F)}=m-|F|}} \prod_{i=1}^{j(F)} c_{m_i}\left(x_i^F; G-x, \boldsymbol{w}|_{G-x}\right) \\ &\leqslant w_x \sum_{\varnothing \neq F \subseteq E(x)} w(F) \sum_{\substack{m_1,\dots,m_{j(F)} \geqslant 0\\ m_1+\dots+m_{j(F)}=m-|F|}} \prod_{i=1}^{j(F)} w_{x_i^F} C(m_i,1) \Delta^{m_i} \end{aligned}$$

$$= w_x \sum_{\varnothing \neq F \subseteq E(x)} C\bigl(m - |F|, j(F)\bigr) \Delta^{m-|F|} w(F) \prod_{i=1}^{j(F)} w_{x_i^F}$$

$$\leqslant w_x \sum_{f=1}^{m} C(m-f, f) \Delta^{m-f} \sum_{\substack{F \subseteq E(x) \\ |F|=f}} \prod_{e = x x_i^F \in F} w_e w_{x_i^F} \tag{5.13}$$

where the second line used the induction hypothesis (5.4) applied to the graph $G - x$ (note that $m_i < m$) and the fact that $d(v; G - x, \boldsymbol{w}|_{G-x}) \leqslant \Delta$ for all $v \in V - x$; the third line used the identity (5.9); and the last line used $j(F) \leqslant |F|$, the fact that $C(m, k)$ is an increasing function of k, and the hypothesis that either $w_{x_i^F} \geqslant 1$ for all $1 \leqslant i \leqslant j(F)$ or G is simple. Using Lemma 5.3, we have

$$c_m(x) \leqslant w_x \Delta^m \sum_{f=1}^{m} \frac{(d/\Delta)^f}{f!} C(m-f, f)$$

$$= w_x \Delta^m \sum_{f=0}^{m} \frac{(d/\Delta)^f}{f!} C(m-f, f)$$

$$= w_x C(m, d/\Delta) \Delta^m, \tag{5.14}$$

where the second line used $C(m, 0) = 0$ for $m \geqslant 1$, and the last line used identity (5.10) with $\kappa = z = d/\Delta$. This proves (5.6). $\square$

We now combine Proposition 5.1 with the extended Penrose inequalities from Section 4:

Proposition 5.4. *Let $G = (V, E)$ be a loopless graph equipped with complex edge weights $\boldsymbol{w} = \{w_e\}_{e \in E}$. Let $x \in V$ and let n be a positive integer. Then*

$$\sum_{\substack{S \ni x \\ S \subseteq V \\ |S| = n}} \bigl|C_{G[S]}(\boldsymbol{w})\bigr| \leqslant \frac{n^{n-1}}{n!} \hat{\Delta}(G, \boldsymbol{w})^{n-1} \prod_{e \in E(x)} \max\bigl\{1, |1 + w_e|\bigr\}^{1/2} \tag{5.15}$$

where $\hat{\Delta}(G, \boldsymbol{w})$ is defined in (1.5). Furthermore, if G is simple, then

$$\sum_{\substack{S \ni x \\ S \subseteq V \\ |S| = n}} \bigl|C_{G[S]}(\boldsymbol{w})\bigr| \leqslant \frac{\Delta^*(G, \boldsymbol{w})}{(n-1)!} \bigl[\Delta^*(G, \boldsymbol{w}) + (n-1)\hat{\Delta}(G, \boldsymbol{w})\bigr]^{n-2} \tag{5.16}$$

where $\Delta^*(G, \boldsymbol{w})$ is defined in (1.9).

Proof. We first prove (5.15). Construct a nonnegative real weight function $\hat{\boldsymbol{w}}$ on $V \cup E$ by putting $\hat{w}_y = \prod_{e \in E(y)} \max\{1, |1 + w_e|\}^{1/2}$ for all $y \in V$, and $\hat{w}_e = |w'_e|$ for all $e \in E$, where w'_e is defined in (4.7). For $y \in S \subseteq V$ let $E(y; G[S])$ denote the set of edges of $G[S]$ incident on y. By bound (4.6b) of Proposition 4.3, we have

$$\sum_{\substack{S \ni x \\ S \subseteq V \\ |S| = n}} \bigl|C_{G[S]}(\boldsymbol{w})\bigr| \leqslant \sum_{\substack{S \ni x \\ S \subseteq V \\ |S| = n}} T_{G[S]}\bigl(|\boldsymbol{w}'|\bigr) \prod_{y \in S} \prod_{e \in E(y; G[S])} \max\bigl\{1, |1 + w_e|\bigr\}^{1/2} \tag{5.17a}$$

$$\leqslant c_{n-1}(x; G, \hat{\boldsymbol{w}}) \tag{5.17b}$$

since the n-vertex trees are a subset of the connected graphs with $n-1$ edges, and $E(y; G[S]) \subseteq E(y)$. Inequality (5.15) now follows by applying Proposition 5.1, using the fact that $d(x; G, \hat{\boldsymbol{w}})$ and $\Delta(G-x, \hat{\boldsymbol{w}}|_{G-x})$ are both bounded above by $\Delta(G, \hat{\boldsymbol{w}}) = \hat{\Delta}(G, \boldsymbol{w})$.

We next prove (5.16). Construct a weight function $\boldsymbol{w}^*$ on $V \cup E$ by putting $w_x^* = 1$, $w_y^* = \prod_{e \in E(y)} \max\{1, |1+w_e|\}^{1/2}$ for all $y \in V \setminus \{x\}$, and $w_e^* = |\tilde{w}_e^{[x]}|$ for all $e \in E$, where $\tilde{w}_e^{[x]}$ is defined in (4.12). By bound (4.10b) of Proposition 4.4, we have

$$\sum_{\substack{S \ni x \\ S \subseteq V \\ |S|=n}} \bigl|C_{G[S]}(\boldsymbol{w})\bigr| \leqslant \sum_{\substack{S \ni x \\ S \subseteq V \\ |S|=n}} T_{G[S]}\bigl(\bigl|\tilde{\boldsymbol{w}}^{[x]}\bigr|\bigr) \prod_{y \in S \setminus \{x\}} \prod_{e \in E(y; G[S])} \max\bigl\{1, |1+w_e|\bigr\}^{1/2} \tag{5.18a}$$

$$\leqslant c_{n-1}\bigl(x; G, \boldsymbol{w}^*\bigr) \tag{5.18b}$$

by the same reasoning as before. Inequality (5.16) now follows by applying Proposition 5.1, using the facts that $d(x; G, \boldsymbol{w}^*) \leqslant \Delta^*(G, \boldsymbol{w})$ and $\Delta(G-x, \boldsymbol{w}^*|_{G-x}) \leqslant \hat{\Delta}(G, \boldsymbol{w})$. $\square$

6. Proof of Theorems 1.2 and 1.3 and Lemma 1.4

We can now put together the results of the preceding sections to prove Theorems 1.2 and 1.3. At the end of this section we will also prove Lemma 1.4.

We begin by stating an analytic lemma that will be needed in proving the equivalence between the various versions (1.7a)–(1.7d) and (1.10a)–(1.10c) of our bounds. To avoid disrupting the flow of the argument, the proof of this lemma is deferred to Appendix A.

Lemma 6.1. *For $\lambda \geqslant 0$ and $\beta > 0$, define the function*

$$F_\lambda(\beta) = \min\left\{L\colon \inf_{\alpha > 0} \bigl(e^\alpha - 1\bigr)^{-1} \sum_{n=2}^{\infty} e^{\alpha n} L^{-(n-1)} \frac{[1+(n-1)\lambda]^{n-2}}{(n-1)!} \leqslant \beta\right\}. \tag{6.1}$$

Then

$$F_\lambda(\beta) = \min_{1<y<1+\beta} \frac{\beta y^\lambda}{(1+\beta-y)\log y}. \tag{6.2}$$

Moreover,

$$F_1(\beta) = \beta W\left(\frac{e}{1+\beta}\right) \Big/ \left[1 - W\left(\frac{e}{1+\beta}\right)\right]^2 \tag{6.3}$$

where W is the Lambert W function [11], i.e. the inverse function to $x \mapsto xe^x$. Finally, for $0 \leqslant \lambda \leqslant 1$ we have

$$F_\lambda(\beta) \leqslant 4\beta^{-1} + (1+2\lambda). \tag{6.4}$$

Proof of Theorem 1.2. We want to show that $Z_G(q, \boldsymbol{w}) \neq 0$ whenever $|q| \geqslant \hat{\mathcal{K}}(\Psi(G, \boldsymbol{w}))\hat{\Delta}(G, \boldsymbol{w})$. We will do this by verifying the condition (3.4) for the polymer weights (2.4), which we recall are

$$\xi(S) = q^{-(|S|-1)} C_{G[S]}(\boldsymbol{w}) \quad \text{for } |S| \geqslant 2. \tag{6.5}$$

By inequality (5.15) of Proposition 5.4, for each $x \in V$ and each $n \geqslant 1$ we have

$$\sum_{\substack{S \ni x \\ S \subseteq V \\ |S|=n}} \bigl|C_{G[S]}(\boldsymbol{w})\bigr| \leqslant \frac{n^{n-1}}{n!} \hat{\Delta}(G, \boldsymbol{w})^{n-1} \prod_{e \in E(x)} \max\bigl\{1, |1+w_e|\bigr\}^{1/2} \tag{6.6a}$$

$$\leqslant \frac{n^{n-1}}{n!} \hat{\Delta}(G, \boldsymbol{w})^{n-1} \Psi(G, \boldsymbol{w})^{1/2}. \tag{6.6b}$$

Therefore, the condition (3.4) for the weights (2.4)/(6.5) is verified as soon as

$$\inf_{\alpha>0}\bigl(e^{\alpha}-1\bigr)^{-1}\sum_{n=2}^{\infty} e^{\alpha n}|q|^{-(n-1)}\frac{n^{n-1}}{n!}\hat{\Delta}(G,\boldsymbol{w})^{n-1}\Psi(G,\boldsymbol{w})^{1/2}\leqslant 1. \tag{6.7}$$

If we set $L=|q|\hat{\Delta}(G,\boldsymbol{w})^{-1}$ and $\psi=\Psi(G,\boldsymbol{w})$ in (6.7), this is precisely the inequality contained in the right-hand side of (1.7a). So $Z_G(q,\boldsymbol{w})\neq 0$ whenever $L\geqslant\hat{\mathcal{K}}(\Psi(G,\boldsymbol{w}))$, i.e. whenever $|q|\geqslant\hat{\mathcal{K}}(\Psi(G,\boldsymbol{w}))\hat{\Delta}(G,\boldsymbol{w})$, where $\hat{\mathcal{K}}(\psi)$ is defined by (1.7a). The equivalence of (1.7a) with (1.7b), (1.7c) and the inequality (1.7d) follow from Lemma 6.1 once we observe that $\hat{\mathcal{K}}(\psi)=F_1(\psi^{-1/2})$. □

Proof of Theorem 1.3. We modify the proof of Theorem 1.2 by using (5.16) in place of (5.15).

Since G is simple, it follows from (5.16) that for each $x\in V$ and each $n\geqslant 1$ we have

$$\begin{aligned}\sum_{\substack{S\ni x\\ S\subseteq V\\ |S|=n}}\bigl|C_{G[S]}(\boldsymbol{w})\bigr| &\leqslant \frac{\Delta^*(G,\boldsymbol{w})}{(n-1)!}\bigl[\Delta^*(G,\boldsymbol{w})+(n-1)\hat{\Delta}(G,\boldsymbol{w})\bigr]^{n-2}\\ &=\Delta^*(G,\boldsymbol{w})^{n-1}\frac{[1+(n-1)\mu]^{n-2}}{(n-1)!}\end{aligned} \tag{6.8}$$

where $\mu=\hat{\Delta}(G,\boldsymbol{w})/\Delta^*(G,\boldsymbol{w})$. Therefore, the condition (3.4) for the weights (2.4)/(6.5) is verified as soon as

$$\inf_{\alpha>0}\bigl(e^{\alpha}-1\bigr)^{-1}\sum_{n\geqslant 2} e^{\alpha n}\bigl[|q|^{-1}\Delta^*(G,\boldsymbol{w})\bigr]^{n-1}\frac{[1+(n-1)\mu]^{n-2}}{(n-1)!}\leqslant 1. \tag{6.9}$$

If we set $L=|q|\Delta^*(G,\boldsymbol{w})^{-1}$, this is precisely the inequality contained in the right-hand side of (1.10a). So $Z_G(q,\boldsymbol{w})\neq 0$ whenever $L\geqslant K^*_{\mu}$, i.e. whenever $|q|\geqslant K^*_{\mu}\Delta^*(G,\boldsymbol{w})$, where $K^*_{\mu}=F_{\mu}(1)$ is defined by (1.10a). The equivalence of (1.10a) with (1.10b) and the inequality (1.10c) then follow from Lemma 6.1. □

Discussion. 1. We can now understand why the apparently minor improvement from (4.6b) to (4.10b) leads to the significant improvement (in most cases) of the final bound from Theorem 1.2 to Theorem 1.3, namely, replacing a growth $\sim\Psi(G,\boldsymbol{w})^{1/2}$ by 1. Indeed, we can see using Lemma 6.1 that whenever we have a bound of the form

$$\sum_{\substack{S\ni x\\ |S|=n}}\bigl|C_{G[S]}(\boldsymbol{w})\bigr|\leqslant\frac{[1+\lambda(n-1)]^{n-2}}{(n-1)!}D^{n-1}\Psi^{b}, \tag{6.10}$$

we will obtain a bound on the roots of $Z_G(q,\boldsymbol{w})$ of the form

$$|q|<DF_{\lambda}\bigl(\Psi^{-b}\bigr). \tag{6.11}$$

The bound (4.6b) gives rise to inequality (5.15), which in turn allows us to deduce Theorem 1.2 by taking $D=\hat{\Delta}$, $\lambda=1$ and $b=1/2$. On the other hand, the bound (4.10b) gives inequality (5.16), which allows us to deduce Theorem 1.3 by taking $D=\Delta^*$, $\lambda=\hat{\Delta}/\Delta^*$ and $b=0$.

2. Let us compare the bounds provided by Theorems 1.2 and 1.3:

$$\text{Theorem 1.2:}\quad \hat{\mathcal{K}}\bigl(\Psi(G,\boldsymbol{w})\bigr)\hat{\Delta}(G,\boldsymbol{w}), \tag{6.12a}$$

$$\text{Theorem 1.3:}\quad K^*_{\mu}\Delta^*(G,\boldsymbol{w}) \tag{6.12b}$$

where $\mu=\hat{\Delta}(G,\boldsymbol{w})/\Delta^*(G,\boldsymbol{w})\in(0,1]$. Their ratio is therefore

$$\frac{\text{Theorem 1.3}}{\text{Theorem 1.2}}=\frac{K^*_{\mu}}{\mu\hat{\mathcal{K}}(\Psi(G,\boldsymbol{w}))}=\frac{F_{\mu}(1)}{\mu F_1(\Psi(G,\boldsymbol{w})^{-1/2})}. \tag{6.13}$$

Now, it is not difficult to see that $\Delta^*(G, \boldsymbol{w}) \leqslant \hat{\Delta}(G, \boldsymbol{w})\Psi(G, \boldsymbol{w})^{1/2}$, or in other words $\Psi(G, \boldsymbol{w})^{-1/2} \leqslant \mu$.[9] Since $F_1(\beta)$ is a decreasing function of β (see Proposition A.1(a) in Appendix A), we have $F_1(\Psi(G, \boldsymbol{w})^{-1/2}) \geqslant F_1(\mu)$ and hence

$$\frac{\text{Theorem 1.3}}{\text{Theorem 1.2}} \leqslant \frac{F_\mu(1)}{\mu F_1(\mu)} \equiv g(\mu). \tag{6.14}$$

Both $F_\mu(1)$ and $\mu F_1(\mu)$ are increasing functions of μ [see Proposition A.1(a), (b)], but their ratio $g(\mu)$ does not have any obvious monotonicity. *Numerically* we find that $g(\mu)$ decreases from the value $K_0^*/4 \approx 1.223222$ at $\mu = 0$ to a minimum value ≈ 0.930714 at $\mu \approx 3.70249$, and then increases to 1 as $\mu \to \infty$. We have not succeeded in *proving* that $g(\mu) \leqslant g(0)$ for $\mu \in [0, 1]$, but if is true we can conclude that Theorem 1.3 is never more than a factor ≈ 1.223222 worse than Theorem 1.2. In any case we have

$$g(\mu) \leqslant \frac{F_1(1)}{\lim_{\mu\to 0} \mu F_1(\mu)} = \frac{K_1^*}{4} \approx 1.726913 \quad \text{for } \mu \in [0, 1]. \tag{6.15}$$

We shall see in Examples 7.1 and 7.2 that Theorem 1.3 can indeed be up to a factor ≈ 1.223222 worse than Theorem 1.2.

3. It is curious that the bound of Theorem 1.3 is not always better than that of Theorem 1.2, despite using a better "ingredient" in its proof: namely, the bound (4.10b) from Proposition 4.4 always beats the bound (4.6b) from Proposition 4.3. How is it that the final result can sometimes be worse?

The explanation is that the ratio of the bounds (4.10b) and (4.6b)

$$\frac{(4.10\text{b})}{(4.6\text{b})} = \frac{T_H(|\tilde{\boldsymbol{w}}^{[x]}|)}{T_H(|\boldsymbol{w}'|) \prod_{e\in \mathrm{E}(x)} \max\{1, |1 + w_e|\}^{1/2}} \tag{6.16}$$

is the product of a "good" factor $\prod_{e\in \mathrm{E}(x)} \max\{1, |1 + w_e|\}^{-1/2}$ and a "bad" factor $T_H(|\tilde{\boldsymbol{w}}^{[x]}|)/T_H(\boldsymbol{w}')$. Now, the "bad" factor $T_H(|\tilde{\boldsymbol{w}}^{[x]}|)/T_H(|\boldsymbol{w}'|)$ is always bounded by $\prod_{e\in \mathrm{E}(x)} \max\{1, |1 + w_e|\}^{1/2}$ – which is why (4.10b) is always better than (4.6b) – so it follows that

$$\frac{\sum_{S\ni x,\, |S|=n} T_{G[S]}(|\tilde{\boldsymbol{w}}^{[x]}|)}{\sum_{S\ni x,\, |S|=n} T_{G[S]}(|\boldsymbol{w}'|)} \leqslant \prod_{e\in \mathrm{E}(x)} \max\bigl\{1, |1 + w_e|\bigr\}^{1/2} \leqslant \Psi(G, \boldsymbol{w})^{1/2}. \tag{6.17}$$

But there is no guarantee that the *upper bounds* on the numerator and denominator of (6.17), obtained by applying respectively the bounds (6.6b) and (6.8), will also have a ratio $\leqslant \Psi(G, \boldsymbol{w})^{1/2}$. Indeed, it can happen that this *fails* (see Examples 7.1 and 7.2).

It is, nevertheless, somewhat disconcerting that Theorem 1.3 is not always better than Theorem 1.2. It would be nice to find a single natural bound that simultaneously improves Theorems 1.2 and 1.3.

Finally, let us prove Lemma 1.4 concerning the behavior of $\Psi(G, \boldsymbol{w})$ and $\hat{\Delta}(G, \boldsymbol{w})$ under parallel reduction:

Proof of Lemma 1.4. Inequality (1.11) follows immediately from the fact that $(1 + w_1)(1 + w_2) = 1 + w_3$. To prove (1.12), let us consider the following cases:

[9] **Proof.** For each edge $e = xy$ we have

$$\begin{aligned} \min\biggl\{|w_e|, \frac{|w_e|}{|1 + w_e|^{1/2}}\biggr\} &= \min\biggl\{|w_e|, \frac{|w_e|}{|1 + w_e|}\biggr\} \times \max\bigl\{1, |1 + w_e|\bigr\}^{1/2} \\ &\leqslant \min\biggl\{|w_e|, \frac{|w_e|}{|1 + w_e|}\biggr\} \times \Psi(G, \boldsymbol{w})^{1/2}. \end{aligned}$$

Multiplying this by $\prod_{f\ni y} \max\{1, |1 + w_f|\}^{1/2}$, summing over $e \ni x$, and taking the maximum over $x \in V$, we obtain the desired inequality. $\square$

Case 1: $|1+w_1| \leqslant 1$ and $|1+w_2| \leqslant 1$. Then $\min\{|w_i|, \frac{|w_i|}{|1+w_i|}\} = |w_i|$ for $1 \leqslant i \leqslant 3$, so we just have to prove that $|w_3| \leqslant |w_1| + |w_2|$. Since $w_3 = w_1 + w_2 + w_1 w_2$, we have

$$\begin{aligned} |w_3| &= |w_1 + w_2 + w_1 w_2| = \bigl|w_1 + w_2(1+w_1)\bigr| \leqslant |w_1| + \bigl|w_2(1+w_1)\bigr| \\ &= |w_1| + |w_2||1+w_1| \leqslant |w_1| + |w_2| \end{aligned} \tag{6.18}$$

since $|1+w_1| \leqslant 1$.

Case 2: $|1+w_1| \geqslant 1$ and $|1+w_2| \geqslant 1$. Then $\min\{|w_i|, \frac{|w_i|}{|1+w_i|}\} = \frac{|w_i|}{|1+w_i|}$ for $1 \leqslant i \leqslant 3$. Let $w_i' = -\frac{w_i}{1+w_i}$ for $1 \leqslant i \leqslant 3$, so that $1 + w_i' = (1+w_i)^{-1}$ for $1 \leqslant i \leqslant 3$ and hence $(1+w_1')(1+w_2') = 1 + w_3'$. Since $|1+w_1'| \leqslant 1$ and $|1+w_2'| \leqslant 1$, we may apply Case 1 to w_1', w_2', w_3' to deduce that $|w_3'| \leqslant |w_1'| + |w_2'|$, as required.

Case 3: $|1+w_1| \leqslant 1$, $|1+w_2| \geqslant 1$ and $|1+w_1||1+w_2| \leqslant 1$. Then $\min\{|w_i|, \frac{|w_i|}{|1+w_i|}\} = |w_i|$ for $i \in \{1,3\}$, and $\min\{|w_2|, \frac{|w_2|}{|1+w_2|}\} = \frac{|w_2|}{|1+w_2|}$. By hypothesis we have $|1+w_1| \leqslant |1+w_2|^{-1}$. Hence

$$|w_3| = \bigl|w_1 + w_2(1+w_1)\bigr| \leqslant |w_1| + |w_2||1+w_1| \leqslant |w_1| + \frac{|w_2|}{|1+w_2|}, \tag{6.19}$$

as required.

Case 4: $|1+w_1| \leqslant 1$, $|1+w_2| \geqslant 1$ and $|1+w_1||1+w_2| \geqslant 1$. Then $\min\{|w_1|, \frac{|w_1|}{|1+w_1|}\} = |w_1|$, and $\min\{|w_i|, \frac{|w_i|}{|1+w_i|}\} = \frac{|w_i|}{|1+w_i|}$ for $i \in \{2,3\}$. Let $w_i' = -\frac{w_i}{1+w_i}$ for $1 \leqslant i \leqslant 3$. Then $|1+w_1'| \geqslant 1$ and $|1+w_2'| \leqslant 1$ with $|1+w_1'||1+w_2'| \leqslant 1$, so we may apply Case 3 (with indices 1 and 2 interchanged) to deduce that $|w_3'| \leqslant \frac{|w_1'|}{|1+w_1'|} + |w_2'| = |w_1| + |w_2'|$, as required. $\square$

Remark. We suspect that the transformation

$$w' = -\frac{w}{1+w} \tag{6.20}$$

employed in Cases 2 and 4, which satisfies $(1+w') = (1+w)^{-1}$ and hence preserves the parallel-connection law $(1+w_1)(1+w_2) = 1+w_3$, may have other applications in the study of the multivariate Tutte polynomial. This transformation is involutive [i.e. $(w')' = w$], maps the complex antiferromagnetic regime $|1+w| \leqslant 1$ onto the complex ferromagnetic regime $|1+w'| \geqslant 1$ and vice versa, and maps the real antiferromagnetic regime $-1 \leqslant w \leqslant 0$ onto the real ferromagnetic regime $0 \leqslant w' \leqslant +\infty$ and vice versa. In the physicists' notation $w = e^J - 1$ where J is the Potts-model coupling, the transformation (6.20) takes the simple form $J' = -J$, which makes its properties obvious.

7. Examples

In this section we examine some examples that shed light on the extent to which Theorems 1.2 and 1.3 are sharp or non-sharp. For each weighted graph $(G, \boldsymbol{w})$, we attempt to compute or estimate the quantity

$$Q_{\max}(G, \boldsymbol{w}) = \max\bigl\{|q|\colon\ Z_G(q, \boldsymbol{w}) = 0\bigr\} \tag{7.1}$$

and compare it to the upper bounds given by Theorems 1.2 and 1.3. In what follows we abbreviate $\hat{\Delta}(G, \boldsymbol{w})$, $\Delta^*(G, \boldsymbol{w})$, $\Psi(G, \boldsymbol{w})$, $Q_{\max}(G, \boldsymbol{w})$ by $\hat{\Delta}$, Δ^*, Ψ, $Q_{\max}$.

Example 7.1. Let $G = K_2$, where the single edge has weight w. Then $Z_{K_2}(q, w) = q(q+w)$, so that $Q_{\max} = |w|$. On the other hand, if $|1+w| \geqslant 1$ we have $\hat{\Delta} = |w|/|1+w|^{1/2}$, $\Delta^* = |w|$, $\Psi = |1+w|$ and $\mu = \hat{\Delta}/\Delta^* = 1/|1+w|^{1/2}$. Theorem 1.2 gives the bound $|q| < \hat{\mathcal{K}}(\Psi)\hat{\Delta}$, which behaves like $4|w|$ as $|w| \to \infty$, while Theorem 1.3 gives the bound $|q| < K_\mu^* \Delta^*$, which behaves like $K_0^*|w| \approx 4.892888|w|$ as $|w| \to \infty$. So Theorem 1.2 is off by a factor of 4 from the truth, while Theorem 1.3 is off by a factor of ≈ 4.892888 from the truth. In particular, Theorem 1.3 is worse than Theorem 1.2 by a factor tending to $K_0^*/4 \approx 1.223222$.

For the special case of $G = K_2$, the convergence conditions (6.7) and (6.9), which were used in the proofs of Theorems 1.2 and 1.3, respectively, become

$$\inf_{\alpha>0} \left(e^{\alpha} - 1\right)^{-1} e^{2\alpha} |q|^{-1} \hat{\Delta}(G, \boldsymbol{w}) \Psi(G, \boldsymbol{w})^{1/2} \leqslant 1, \tag{7.2}$$

$$\inf_{\alpha>0} \left(e^{\alpha} - 1\right)^{-1} e^{2\alpha} |q|^{-1} \Delta^*(G, \boldsymbol{w}) \leqslant 1 \tag{7.3}$$

because the only polymer in the graph K_2 has size $n = 2$. Since $\hat{\Delta}(G, \boldsymbol{w})\Psi(G, \boldsymbol{w})^{1/2} = \Delta^*(G, \boldsymbol{w}) = |w|$, we have

$$(7.2) \iff (7.3) \iff |q| \geqslant 4|w|, \tag{7.4}$$

which differs from the truth $Q_{\max} = |w|$ by a factor of 4. We can understand this behavior as follows:

(1) The lost factor of 4 comes from the fact that, for a polymer gas consisting of a single polymer S of cardinality $|S| = 2$, the Gruber–Kunz–Fernández–Procacci condition (Proposition 3.1) gives $\Xi \neq 0$ whenever $|\rho(S)| \leqslant 1/4$, whereas the truth is that $\Xi \neq 0$ whenever $|\rho(S)| < 1$.

(2) Though the convergence condition (6.7) involves a sum $\sum_{n=2}^{\infty}$, the terms for $n > 2$ make a negligible contribution in the limit $|w| \to \infty$ because

$$|q|^{-(n-1)} \hat{\Delta}(G, \boldsymbol{w})^{n-1} \Psi(G, \boldsymbol{w})^{1/2} = \left(|w|/|q|\right)^{n-1} |1 + w|^{-(n-2)/2}, \tag{7.5}$$

which tends to zero as $|w| \to \infty$ whenever $|q| \geqslant \text{const} \times |w|$ and $n > 2$. That is why Theorem 1.2 is off from the truth by the *same* factor 4 that we see in (7.4), despite the fact that its proof allows for arbitrarily large polymers that do not occur when $G = K_2$.

(3) By contrast, in the convergence condition (6.9), the terms with $n > 2$ do *not* disappear in the limit $|w| \to \infty$ with $|q|$ of order $|w|$, because

$$\left[|q|^{-1} \Delta^*(G, \boldsymbol{w})\right]^{n-1} = \left(|w|/|q|\right)^{n-1} \tag{7.6}$$

is of order 1 for all n. This is why Theorem 1.3 is off from the truth by *more* than the factor 4 that we see in (7.4); we lose an additional factor $K_0^*/4 \approx 1.223222$ by allowing for nonexistent large polymers.

Example 7.2. In *any* simple graph G with at least one edge, we can choose weights $\boldsymbol{w}$ such that Theorem 1.2 beats Theorem 1.3 by a factor arbitrarily close to $K_0^*/4 \approx 1.223222$. It suffices to take $w_e = w$ (with $|1 + w| \geqslant 1$) on all the edges of a nonempty matching, and $w_e = w_0$ on all other edges; then as $w_0 \to 0$ we have $Q_{\max} \to |w|$, $\hat{\Delta} \to |w|/|1 + w|^{1/2}$, $\Delta^* \to |w|$, $\Psi \to |1 + w|$ and $\mu = \hat{\Delta}/\Delta^* \to 1/|1 + w|^{1/2}$. So the comparison of the bounds is the same as for $G = K_2$, and Theorem 1.2 beats Theorem 1.3 by a factor tending to $K_0^*/4 \approx 1.223222$ as $|w| \to \infty$.

For instance, let G be the n-cycle C_n with $n \geqslant 3$, taking $w_e = w$ for exactly one edge and $w_e = w_0$ for all other edges. Then $Z_G(q, w) = (q + w)(q + w_0)^{n-1} + w w_0^{n-1}(q - 1)$. As $|w| \to \infty$ at fixed n and w_0, we have $Q_{\max}(G, \boldsymbol{w}) = |w| + o(|w|)$. On the other hand, if $|1 + w_0| \geqslant 1$ and $|w| \gg |w_0|$ we have $\hat{\Delta}(G, \boldsymbol{w}) = |w_0| + |1 + w_0|^{1/2}|w|/|1 + w|^{1/2}$, $\Delta^*(G, \boldsymbol{w}) = |w_0||1 + w_0|^{1/2} + |1 + w_0|^{1/2}|w|$ and $\Psi(G, \boldsymbol{w}) = |1 + w_0||1 + w|$. Therefore, as $|w| \to \infty$ the bounds of Theorems 1.2 and 1.3 are $4|1 + w_0||w| + O(|w|^{1/2})$ and $K_0^*|1 + w_0|^{1/2}|w| + O(1)$, respectively, where $K_0^* \approx 4.892888$. Both of these bounds have the correct order of magnitude as $|w| \to \infty$ at fixed n and w_0, but are off by a constant factor ($4|1 + w_0|$ or $K_0^*|1 + w_0|^{1/2}$, respectively). The bound given by Theorem 1.2 is better than that given by Theorem 1.3 when $|1 + w_0|$ is small, and worse when $|1 + w_0|$ is large.

Example 7.3. Let $G = K_2^{(k)}$ (a pair of vertices connected by k parallel edges) with $w_e = w$ for all e. Then $Z_G(q, w) = q[q + (1 + w)^k - 1]$, so $Q_{\max}(G, \boldsymbol{w}) = |(1 + w)^k - 1|$. Now, if $|1 + w| \geqslant 1$ we have $\hat{\Delta}(G, \boldsymbol{w}) = k|w||1 + w|^{\frac{k}{2}-1}$ and $\Psi(G, \boldsymbol{w}) = |1 + w|^k$. Therefore, as $|w| \to \infty$ at fixed k, the bound of Theorem 1.2 is a factor $4k$ from being sharp.

On the other hand, we may first apply parallel reduction to yield a simple graph $\hat{G} = K_2$ with weight $\hat{w} = (1+w)^k - 1$ on its single edge, and then apply Theorem 1.2 or 1.3 to $(\hat{G}, \hat{\boldsymbol{w}})$. The resulting bound is then (as $|w| \to \infty$) a factor 4 or ≈ 4.892888 from being sharp (see Example 7.1).

Example 7.4. Let G be the n-cycle C_n (which is simple for $n \geqslant 3$), with $w_e = w$ for all e. Then $Z_G(q, w) = (q+w)^n + (q-1)w^n$. As $|w| \to \infty$ at fixed n, we have $Q_{\max}(G, \boldsymbol{w}) = |w|^{n/(n-1)} + O(|w|)$. On the other hand, if $|1+w| \geqslant 1$ we have $\hat{\Delta} = 2|w|$, $\Delta^* = 2|w||1+w|^{1/2}$ and $\Psi = |1+w|^2$. Therefore, as $|w| \to \infty$ the bounds of Theorems 1.2 and 1.3 are $8|w|^2 + O(|w|)$ and $2K_0^*|w|^{3/2} + O(|w|)$, respectively (here $2K_0^* \approx 9.785776$). Both of these bounds have the wrong order of magnitude as $|w| \to \infty$ at fixed $n \geqslant 4$, but the bound given by Theorem 1.3 is a significant improvement over that given by Theorem 1.2. $\square$

Example 7.5. Let G be the complete graph K_n. Take $w_e = w > 0$ for all e, with w fixed independent of n (unlike the usual [8] scaling $w = \lambda/n$). Then Janson [18] has very recently proven that

$$\lim_{n\to\infty} \frac{1}{n^2} \log Z_{K_n}\big(e^{\alpha n}, w\big) = \max\left[\frac{1}{2}\log(1+w), \alpha\right] \quad \text{for } \alpha \geqslant 0. \tag{7.7}$$

[This is because the sum (1.1) is dominated by two contributions: the terms with (V, A) connected, which together contribute $e^{\alpha n}(1+w)^{\binom{n}{2}}[1+o(1)]$, and the term $A = \varnothing$, which contributes $e^{\alpha n^2}$.] It then follows from the Yang–Lee [36] theory of phase transitions (see e.g. [29, Theorem 3.1]) that $Z_{K_n}(e^{\alpha n}, w)$ must have complex roots α_n that converge to $\alpha_\star = \frac{1}{2}\log(1+w)$ as $n \to \infty$. Hence $Q_{\max}(K_n, \boldsymbol{w}) \geqslant (1+w)^{n/2+o(n)}$ (and this is presumably the actual order of magnitude). On the other hand, we have $\Delta^*(K_n, \boldsymbol{w}) = (n-1)w(1+w)^{n/2-1}$, so that the upper bound given by Theorem 1.3 is nearly sharp when $n \to \infty$ at fixed $w > 0$ [it exceeds the truth by at most a factor $e^{o(n)}$ even though both the truth and the bound are growing exponentially in n].

By contrast, $\hat{\Delta} = (n-1)w(1+w)^{(n-3)/2}$ and $\Psi = (1+w)^{n-1}$, so the bound of Theorem 1.2 is much worse because of its growth as $(1+w)^{n-2}$ rather than $(1+w)^{n/2-1}$.

Example 7.6. Let G be a large finite piece of the simple hypercubic lattice $\mathbb{Z}^d$ (for some fixed $d \geqslant 2$) with nearest-neighbor edges, and take $w_e = w > 0$ for all e. For real $q > 0$ sufficiently large, it is known [24,23,20,22,10] that the first-order phase-transition point w_t lies at

$$w_t(q) = q^{1/d} + O(1). \tag{7.8}$$

It then follows from the Yang–Lee [36] theory of phase transitions that there will be complex zeros of the partition function arbitrarily close (as G grows) to the phase-transition point $(q, w_t(q))$; so as $w \uparrow \infty$ (for fixed $d \geqslant 2$) we will have asymptotically $Q_{\max}(G, \boldsymbol{w}) \geqslant w^d[1 + O(1/w)]$ (and this is presumably the actual order of magnitude). Since $\Delta^*(G, \boldsymbol{w}) = 2dw(1+w)^{d-1/2}$, the upper bound given by Theorem 1.3 is off by at most a factor of order $w^{1/2}$ (i.e. it grows as $w^{d+1/2}$ instead of w^d). By contrast, $\hat{\Delta} = 2dw(1+w)^{d-1}$ and $\Psi = (1+w)^{2d}$, so the bound of Theorem 1.2 is again much worse, because it grows as w^{2d} rather than $w^{d+1/2}$.

Example 7.7. Let G be a disjoint union $G = G_1 \uplus G_2$. Then $Q_{\max}(G) = \max\{Q_{\max}(G_1), Q_{\max}(G_2)\}$, $\hat{\Delta}(G) = \max\{\hat{\Delta}(G_1), \hat{\Delta}(G_2)\}$ and $\Psi(G) = \max\{\Psi(G_1), \Psi(G_2)\}$. But the product $\hat{\mathcal{K}}(\Psi)\hat{\Delta}$ for G *can exceed* the maximum of those for G_1 and G_2 because one factor could be maximized for G_1 and the other for G_2. For instance, for $i = 1, 2$ let G_i be an r_i-regular graph with all edge weights equal to w_i, where $|1+w_i| \geqslant 1$. Then

$$\hat{\Delta}(G_i) = r_i|w_i||1+w_i|^{r_i/2-1}, \tag{7.9a}$$

$$\Psi(G_i) = |1+w_i|^{r_i}. \tag{7.9b}$$

Now choose (for instance) $r_1 = \rho \gg 1$, $r_2 = 3$, $w_1 = 1$, $w_2 \gg 1$. Then

$$\frac{\hat{\Delta}(G_1)}{\hat{\Delta}(G_2)} = \frac{\rho 2^{\rho/2-1}}{3w_2(1+w_2)^{1/2}} \approx \frac{\rho 2^{\rho/2}}{6w_2^{3/2}} \tag{7.10}$$

while

$$\frac{\Psi(G_2)}{\Psi(G_1)} = \frac{(1+w_2)^3}{2^\rho} \approx \frac{w_2^3}{2^\rho}. \tag{7.11}$$

So if we choose

$$\rho^2 2^\rho \gg w_2^3 \gg 2^\rho \tag{7.12}$$

we will have $\hat{\Delta}(G_1) \gg \hat{\Delta}(G_2)$ but $\Psi(G_2) \gg \Psi(G_1)$.

Acknowledgments

We are extremely grateful to Svante Janson for answering our query about the behavior of $Z_{K_n}(q, w)$ when $w > 0$ is taken independent of n [cf. (7.7)]. We are also indebted to an anonymous referee, whose incisive comments on the previous version of our paper led us to obtain some notable improvements.

We wish to thank the Isaac Newton Institute for Mathematical Sciences, University of Cambridge, for generous support during the programme on Combinatorics and Statistical Mechanics (January–June 2008), where this work was begun. One of us (A.D.S.) also thanks the Institut Henri Poincaré – Centre Emile Borel for hospitality during the programmes on Interacting Particle Systems, Statistical Mechanics and Probability Theory (September–December 2008) and Statistical Physics, Combinatorics and Probability (September–December 2009), and the Laboratoire de Physique Théorique at the École Normale Supérieure for hospitality during April–June 2011.

This research was supported in part by US National Science Foundation grant PHY–0424082, by the Conselho Nacional de Desenvolvimento Científico e Tecnológico (CNPq), and by the Fundação de Amparo à Pesquisa do Estado de Minas Gerais (FAPEMIG).

Appendix A. Proof of Lemma 6.1 and related facts

In this appendix we prove Lemma 6.1. Actually, we prove much more: though only parts (e), (f), (h) of Proposition A.1 below actually arise in Lemma 6.1 and hence in the proofs of Theorems 1.2 and 1.3, we think it worthwhile to collect here some additional properties of the function $F_\lambda(\beta)$ defined by (A.1). Some of these properties will be invoked in the Discussion after the proof of Theorem 1.3, while others may end up playing a role in future work.

Proposition A.1. *For $\lambda \geqslant 0$ and $\beta > 0$, define the function*

$$F_\lambda(\beta) = \min\left\{L\colon \inf_{\alpha>0}\bigl(e^\alpha - 1\bigr)^{-1} \sum_{n=2}^{\infty} e^{\alpha n} L^{-(n-1)} \frac{[1+(n-1)\lambda]^{n-2}}{(n-1)!} \leqslant \beta\right\}. \tag{A.1}$$

Then:

(a) *$F_\lambda(\beta)$ is an increasing function of λ and a decreasing function of β.*
(b) *$\beta F_\lambda(\beta)$ is an increasing function of both λ and β.*
(c) *$F_\lambda(\mu/\lambda)/\lambda$ is a decreasing function of both λ and μ (> 0). In particular, $F_\lambda(\beta)/\lambda$ is a decreasing function of both λ and β.*
(d) *$\log F_\lambda(\beta)$ is a convex function of $\log \beta$.*
(e) *We have*

$$F_\lambda(\beta) = \min_{1<y<1+\beta} \frac{\beta y^\lambda}{(1+\beta-y)\log y}. \tag{A.2}$$

(f) *For* $\lambda = 0, 1$ *we have*

$$F_0(\beta) = \frac{\beta}{1+\beta} W\big((1+\beta)e\big) / \big[W\big((1+\beta)e\big) - 1\big]^2, \tag{A.3}$$

$$F_1(\beta) = \beta W\left(\frac{e}{1+\beta}\right) \bigg/ \left[1 - W\left(\frac{e}{1+\beta}\right)\right]^2 \tag{A.4}$$

where W *is the Lambert* W *function* [11], *i.e. the inverse function to* $x \mapsto xe^x$.

(g) *For* $0 \leqslant \lambda \leqslant \lambda'$ *we have*

$$F_\lambda(\beta) \leqslant \frac{1+2\lambda}{1+2\lambda'} F_{\lambda'}\left(\frac{1+2\lambda}{1+2\lambda'}\beta\right). \tag{A.5}$$

(h) *For* $0 \leqslant \lambda \leqslant 1$ *we have*

$$F_\lambda(\beta) \leqslant 4\beta^{-1} + (1+2\lambda). \tag{A.6}$$

Proof. (a) It is immediate from the definition (A.1) that $F_\lambda(\beta)$ is increasing in λ and decreasing in β.

(b) The change of variables $L' = \beta L$ in (A.1) shows that

$$\beta F_\lambda(\beta) = \min\left\{L'\colon \inf_{\alpha>0} \big(e^\alpha - 1\big)^{-1} \sum_{n=2}^\infty e^{\alpha n} \big(L'\big)^{-(n-1)} \beta^{n-2} \frac{[1+(n-1)\lambda]^{n-2}}{(n-1)!} \leqslant 1\right\} \tag{A.7}$$

is increasing in both λ and β.

(c) The change of variables $L'' = L/\lambda$ in (A.1) shows that

$$\frac{F_\lambda(\mu/\lambda)}{\lambda} = \min\left\{L''\colon \inf_{\alpha>0} \big(e^\alpha - 1\big)^{-1} \sum_{n=2}^\infty e^{\alpha n} \big(L''\big)^{-(n-1)} \frac{[\lambda^{-1}+(n-1)]^{n-2}}{(n-1)!} \leqslant \mu\right\} \tag{A.8}$$

is decreasing in both λ and μ.

(d) Suppose that we have triplets (α_i, L_i, β_i) satisfying

$$\sum_{n=2}^\infty e^{\alpha_i n} L_i^{-(n-1)} \frac{[1+(n-1)\lambda]^{n-2}}{(n-1)!} \leqslant \beta_i\big(e^{\alpha_i} - 1\big) \tag{A.9}$$

for $i = 1, 2$. Now let $\kappa \in [0, 1]$ and define

$$\bar{\alpha} = \kappa\alpha_1 + (1-\kappa)\alpha_2, \tag{A.10a}$$

$$\bar{L} = L_1^\kappa L_2^{1-\kappa}, \tag{A.10b}$$

$$\bar{\beta} = \beta_1^\kappa \beta_2^{1-\kappa}. \tag{A.10c}$$

Then Hölder's inequality with $p = 1/\kappa$ and $q = 1/(1-\kappa)$ yields

$$\sum_{n=2}^\infty e^{\bar{\alpha} n} \bar{L}^{-(n-1)} \frac{[1+(n-1)\lambda]^{n-2}}{(n-1)!} \leqslant \bar{\beta}\big(e^{\alpha_1} - 1\big)^\kappa \big(e^{\alpha_2} - 1\big)^{1-\kappa}. \tag{A.11}$$

And since the function $\alpha \mapsto \log(e^\alpha - 1)$ is concave on $(0, \infty)$, we have $(e^{\alpha_1} - 1)^\kappa (e^{\alpha_2} - 1)^{1-\kappa} \leqslant e^{\bar{\alpha}} - 1$. This proves (d).

(e) The proof that (A.1) is equivalent to (A.2) will be modelled on an argument of Borgs [9, Eq. (4.22) ff.], who proved a related result.

Note first that $c \mapsto ce^{-c}$ maps the interval $[0,1]$ strictly monotonically onto the interval $[0,1/e]$; and recall [32, p. 28] that its inverse map is the tree function

$$T(x) = \sum_{n=1}^{\infty} \frac{n^{n-1}}{n!} x^n, \tag{A.12}$$

which is convergent and monotonically increasing for $0 \leqslant x \leqslant 1/e$ and satisfies $T(ce^{-c}) = c$ for $0 \leqslant c \leqslant 1$. Moreover, it is well known (see e.g. [11, Eq. (2.36)]) that for all real $\kappa > 0$ one has [cf. (5.8)]

$$\left(\frac{T(z)}{z}\right)^{\kappa} = \sum_{m=0}^{\infty} \frac{\kappa(m+\kappa)^{m-1}}{m!} z^m \tag{A.13}$$

(this is an easy consequence of the Lagrange inversion formula). Writing for convenience $U(z) = T(z)/z$, we therefore have

$$\sum_{n=1}^{\infty} \frac{[1+(n-1)\lambda]^{n-2}}{(n-1)!} z^n = zU(\lambda z)^{1/\lambda} \tag{A.14}$$

for all real $\lambda > 0$.

The inequality on the right-hand side of (A.1) is then equivalent to the statement that $\lambda e^{\alpha}/L \leqslant 1/e$ (otherwise the sum would be divergent) and

$$e^{\alpha} U\big(\lambda e^{\alpha}/L\big)^{1/\lambda} - e^{\alpha} \leqslant \beta\big(e^{\alpha} - 1\big). \tag{A.15}$$

Eliminating L in favor of a new variable c defined by $\lambda e^{\alpha}/L = ce^{-c}$ with $0 \leqslant c \leqslant 1$, and using the fact that $U(ce^{-c}) = e^c$, we see that the inequality on the right-hand side of (A.1) is equivalent to

$$c \leqslant \min\big\{1, \lambda \log\big[1 + \beta\big(1 - e^{-\alpha}\big)\big]\big\}. \tag{A.16}$$

Since $L = \lambda e^{\alpha}/(ce^{-c})$, and ce^{-c} increases monotonically with c for $0 \leqslant c \leqslant 1$, we deduce that (A.16) is equivalent to

$$L \geqslant \begin{cases} \frac{e^{\alpha}[1+\beta(1-e^{-\alpha})]^{\lambda}}{\log[1+\beta(1-e^{-\alpha})]} & \text{if } \beta(1-e^{-\alpha}) \leqslant e^{1/\lambda} - 1, \\ \lambda e^{\alpha+1} & \text{if } \beta(1-e^{-\alpha}) \geqslant e^{1/\lambda} - 1. \end{cases} \tag{A.17}$$

Changing variables from α to $y = 1 + \beta(1 - e^{-\alpha})$, we can rewrite this as

$$L \geqslant \begin{cases} \frac{\beta y^{\lambda}}{(1+\beta-y)\log y} & \text{if } 1 < y < \min(e^{1/\lambda}, 1+\beta), \\ \frac{\lambda\beta e}{1+\beta-y} & \text{if } e^{1/\lambda} \leqslant y < 1+\beta. \end{cases} \tag{A.18}$$

Now we can optimize over y: the minimum will always be found in the interval $1 < y \leqslant e^{1/\lambda}$, so we have

$$F_{\lambda}(\beta) = \min_{1<y<\min(e^{1/\lambda},1+\beta)} \frac{\beta y^{\lambda}}{(1+\beta-y)\log y} = \min_{1<y<1+\beta} \frac{\beta y^{\lambda}}{(1+\beta-y)\log y}, \tag{A.19}$$

where the final equality results from the fact that $y^{\lambda}/[(1+\beta-y)\log y]$ is increasing for $e^{1/\lambda} \leqslant y < 1+\beta$. This proves the equivalence of (A.1) with (A.2) for $\lambda > 0$; and the case $\lambda = 0$ follows by taking limits (or by an easy direct proof).

(f) For $\lambda = 0$, simple calculus shows that the minimum in (A.2) is attained at $y = (1+\beta)/W((1+\beta)e)$, so that $F_0(\beta)$ is given by (A.3). Likewise, for $\lambda = 1$, simple calculus shows that the minimum in (A.2) is attained at $y = (1+\beta)W(e/(1+\beta))$, so that $F_1(\beta)$ is given by (A.4).

(g) To prove the comparison inequality (A.5), it suffices to observe that whenever $0 \leqslant \lambda \leqslant \lambda'$ and $n \geqslant 2$ we have

$$\left(\frac{1+(n-1)\lambda}{1+(n-1)\lambda'}\right)^{n-2} \leqslant \left(\frac{1+2\lambda}{1+2\lambda'}\right)^{n-2} \tag{A.20}$$

(just consider $n = 2$ and $n \geqslant 3$ separately). Inserting this into the definition (A.1) yields (A.5).

(h) To prove the upper bound (A.6), write $y = 1 + x$ in (A.2) and use the inequalities

$$\frac{1}{\log(1+x)} \leqslant \frac{1}{x} + \frac{1}{2}, \tag{A.21}$$

$$(1+x)^{\lambda} \leqslant 1 + \lambda x \tag{A.22}$$

which are valid for all $x > 0$ and $0 \leqslant \lambda \leqslant 1$.[10] Therefore,

$$\frac{\beta y^{\lambda}}{(1+\beta-y)\log y} \leqslant \frac{\beta(1+\lambda x)(\frac{1}{x}+\frac{1}{2})}{\beta - x}. \tag{A.23}$$

The latter function is minimized at $x = (-2 + \sqrt{4 + (2+4\lambda)\beta + 2\lambda\beta^2})/[1 + (2+\beta)\lambda] \in (0, \beta)$, with minimum value

$$\frac{1}{2} + \lambda + \frac{2}{\beta} + \frac{2}{\beta}\sqrt{(1+\beta/2)(1+\lambda\beta)}. \tag{A.24}$$

This, in turn, is bounded above by $4\beta^{-1} + (1+2\lambda)$ on the entire interval $0 < \beta < \infty$.[11] [Alternatively, it suffices to make this proof for $\lambda = 1$ and then invoke (A.5) to deduce the result for $0 \leqslant \lambda < 1$.] $\square$

Remarks. 1. The proof of Proposition A.1(e) becomes a bit simpler for $\beta \leqslant e^{1/\lambda} - 1$, and hence we need not worry about the second case in (A.17) and (A.18). This simplification applies in particular when $\lambda \leqslant 1$ and $\beta \leqslant 1$, which covers what is needed in the proofs of both Theorem 1.2 ($\lambda = 1$, $\beta = \psi^{-1/2} \leqslant 1$) and Theorem 1.3 ($0 < \lambda \leqslant 1$, $\beta = 1$).

2. We can compute the small-β asymptotics of $F_\lambda(\beta)$ by expanding (A.2) in powers of $y - 1$: the minimum is located at

$$y = 1 + \frac{1}{2}\beta - \frac{1+2\lambda}{16}\beta^2 + \frac{5+12\lambda}{192}\beta^3 - \frac{43+122\lambda+12\lambda^2-24\lambda^3}{3072}\beta^4 + \cdots \tag{A.25}$$

and we have

$$F_\lambda(\beta) = 4\beta^{-1} + (1+2\lambda) - \frac{7+12\lambda-12\lambda^2}{48}\beta + \frac{11+26\lambda-12\lambda^2-8\lambda^3}{192}\beta^2 + \cdots. \tag{A.26}$$

For $\lambda = 0, 1$ an alternate method is to expand (A.3)/(A.4): we obtain

$$F_0(\beta) = 4\beta^{-1} + 1 - \frac{7}{48}\beta + \frac{11}{192}\beta^2 - \frac{443}{15\,360}\beta^3 + \frac{607}{36\,864}\beta^4 - \cdots, \tag{A.27}$$

$$F_1(\beta) = 4\beta^{-1} + 3 - \frac{7}{48}\beta + \frac{17}{192}\beta^2 - \frac{923}{15\,360}\beta^3 + \frac{8113}{184\,320}\beta^4 - \cdots. \tag{A.28}$$

[10] **Proof of (A.21).** Write $t = \log(1+x) > 0$; then (A.21) states that $1/t \leqslant 1/(e^t - 1) + 1/2$. This is trivially true for $t \geqslant 2$; and for $0 < t < 2$ it is equivalent to $e^t - 1 \leqslant t/(1 - t/2)$, which is obvious from the Taylor series. $\square$

[11] **Proof.** We have

$$\sqrt{(1+c_1\beta)(1+c_2\beta)} \leqslant 1 + \frac{c_1+c_2}{2}\beta$$

for all $c_1, c_2, \beta \geqslant 0$, as is easily seen by squaring both sides and using the arithmetic–geometric-mean inequality $\sqrt{c_1c_2} \leqslant (c_1+c_2)/2$. $\square$

Therefore, the large-ψ asymptotics of $\hat{\mathcal{K}}(\psi) = F_1(\psi^{-1/2})$ is

$$\hat{\mathcal{K}}(\psi) = 4\psi^{1/2} + 3 - \frac{7}{48}\psi^{-1/2} + \frac{17}{192}\psi^{-1} - \frac{923}{15\,360}\psi^{-3/2} + \frac{8113}{184\,320}\psi^{-2} - \cdots. \tag{A.29}$$

3. In the preprint version of this paper,[12] we conjectured (based on plots of F_1 and its derivatives) that $F_1(\beta)$ is a *completely monotone* function of β on $(0,\infty)$, i.e. $(-1)^k d^k F_1(\beta)/d\beta^k \geqslant 0$ for all $\beta > 0$ and all integers $k \geqslant 0$, and indeed that $G_1(\beta) = F_1(\beta) - 4/\beta$ is completely monotone, which is stronger.[13] Even more strongly, we conjectured (based on computations for $\operatorname{Im}\beta > 0$) that $G_\lambda(\beta) = F_\lambda(\beta) - 4/\beta$ is a *Stieltjes function* for $\lambda = 0$ and $\lambda = 1$, i.e. it can be written in the form

$$f(\beta) = C + \int\limits_{[0,\infty)} \frac{d\rho(t)}{\beta + t} \tag{A.30}$$

where $C \geqslant 0$ and ρ is a positive measure on $[0,\infty)$.[14] This latter conjecture has now been proven by Kalugin, Jeffrey and Corless [19]. It is even possible that G_λ is a Stieltjes function also for $0 < \lambda < 1$, but a different method of proof will be needed.

References

[1] N.I. Akhiezer, The Classical Moment Problem and Some Related Questions in Analysis, translated by N. Kemmer, Hafner, New York, 1965.
[2] C. Berg, The Stieltjes cone is logarithmically convex, in: I. Laine, O. Lehto, T. Sorvali (Eds.), Complex Analysis, Joensuu, 1978, in: Lecture Notes in Math., vol. 747, Springer-Verlag, Berlin, Heidelberg, New York, 1979, pp. 46–54.
[3] C. Berg, Quelques remarques sur le cône de Stieltjes, in: F. Hirsch, G. Mokobodzki (Eds.), Séminaire de Théorie du Potentiel, Paris, No. 5, in: Lecture Notes in Math., vol. 814, Springer-Verlag, Berlin, Heidelberg, New York, 1980, pp. 70–79.
[4] C. Berg, Stieltjes–Pick–Bernstein–Schoenberg and their connection to complete monotonicity, in: J. Mateu, E. Porcu (Eds.), Positive Definite Functions: From Schoenberg to Space–Time Challenges, Dept. of Mathematics, Universitat Jaume I de Castelló, Spain, 2008; also available at http://www.math.ku.dk/~berg/.
[5] N. Biggs, Algebraic Graph Theory, second ed., Cambridge University Press, Cambridge, New York, 1993.
[6] R. Bissacot, R. Fernández, A. Procacci, On the convergence of cluster expansions for polymer gases, J. Stat. Phys. 139 (2010) 598–617, arXiv:1002.3261.
[7] A. Björner, The homology and shellability of matroids and geometric lattices, in: N. White (Ed.), Matroid Applications, in: Encyclopedia Math. Appl., vol. 40, Cambridge University Press, Cambridge, 1992, pp. 226–283 (Chapter 7).
[8] B. Bollobás, G. Grimmett, S. Janson, The random-cluster model on the complete graph, Probab. Theory Related Fields 104 (1996) 283–317.
[9] C. Borgs, Absence of zeros for the chromatic polynomial of bounded degree graphs, Combin. Probab. Comput. 15 (2006) 63–74.
[10] C. Borgs, R. Kotecký, S. Miracle-Solé, Finite-size scaling for Potts models, J. Stat. Phys. 62 (1991) 529–551.
[11] R.M. Corless, G.H. Gonnet, D.E.G. Hare, D.J. Jeffrey, D.E. Knuth, On the Lambert W function, Adv. Comput. Math. 5 (1996) 329–359.
[12] R. Fernández, R. Kotecký, A.D. Sokal, D. Ueltschi, in preparation.
[13] R. Fernández, A. Procacci, Cluster expansion for abstract polymer models: New bounds from an old approach, Comm. Math. Phys. 274 (2007) 123–140, arXiv:math-ph/0605041.
[14] R. Fernández, A. Procacci, Regions without complex zeros for chromatic polynomials on graphs with bounded degree, Combin. Probab. Comput. 17 (2008) 225–238, arXiv:0704.2617 [math-ph].
[15] I.M. Gessel, B.E. Sagan, The Tutte polynomial of a graph, depth-first search, and simplicial complex partitions, Electron. J. Combin. 3 (2) (1996), #R9.
[16] C. Gruber, H. Kunz, General properties of polymer systems, Comm. Math. Phys. 22 (1971) 133–161.
[17] B. Jackson, A.D. Sokal, Maxmaxflow and counting subgraphs, Electron. J. Combin. 17 (1) (2010), #R99, arXiv:math.CO/0703585v2.

[12] http://arxiv.org/abs/0810.4703v2.

[13] See e.g. [33] for the theory of completely monotone functions on $(0,\infty)$ – in particular the Bernstein–Hausdorff–Widder theorem, which states that a function is completely monotone on $(0,\infty)$ if and only if it is the Laplace transform of a positive measure supported on $[0,\infty)$.

[14] More information on Stieltjes functions can be found in [33], [1, pp. 126–128], [2–4,31] and the references cited therein. In order to test numerically the Stieltjes property for $G_0(\beta)$ and $G_1(\beta)$, we have used the complex-analysis characterization: a function $f:(0,\infty) \to \mathbb{R}$ is Stieltjes if and only if it is the restriction to $(0,\infty)$ of an analytic function on the cut plane $\mathbb{C} \setminus (-\infty, 0]$ satisfying $f(z) \geqslant 0$ for $z > 0$ and $\operatorname{Im} f(z) \leqslant 0$ for $\operatorname{Im} z > 0$. See e.g. [1, p. 127] or [3].

[18] S. Janson, private communication, September 2008.
[19] G.A. Kalugin, D.J. Jeffrey, R.M. Corless, Stieltjes, Poisson and other integral representations for functions of Lambert W, preprint, arXiv:1103.5640, March 2011.
[20] R. Kotecký, L. Laanait, A. Messager, J. Ruiz, The q-state Potts model in the standard Pirogov–Sinai theory: Surface tensions and Wilson loops, J. Stat. Phys. 58 (1990) 199–248.
[21] R. Kotecký, D. Preiss, Cluster expansion for abstract polymer models, Comm. Math. Phys. 103 (1986) 491–498.
[22] L. Laanait, A. Messager, S. Miracle-Solé, J. Ruiz, S. Shlosman, Interfaces in the Potts model. I. Pirogov–Sinai theory of the Fortuin–Kasteleyn representation, Comm. Math. Phys. 140 (1991) 81–91.
[23] L. Laanait, A. Messager, J. Ruiz, Phases coexistence and surface tensions for the Potts model, Comm. Math. Phys. 105 (1986) 527–545.
[24] D.H. Martirosian, Translation invariant Gibbs states in the q-state Potts model, Comm. Math. Phys. 105 (1986) 281–290.
[25] O. Penrose, Convergence of fugacity expansions for classical systems, in: T.A. Bak (Ed.), Statistical Mechanics: Foundations and Applications, Benjamin, New York, Amsterdam, 1967, pp. 101–109.
[26] R.B. Potts, Some generalized order-disorder transformations, Proc. Cambridge Philos. Soc. 48 (1952) 106–109.
[27] A.D. Scott, A.D. Sokal, The repulsive lattice gas, the independent-set polynomial, and the Lovász local lemma, J. Stat. Phys. 118 (2005) 1151–1261, arXiv:cond-mat/0309352.
[28] A.D. Sokal, Bounds on the complex zeros of (di)chromatic polynomials and Potts-model partition functions, Combin. Probab. Comput. 10 (2001) 41–77, arXiv:cond-mat/9904146.
[29] A.D. Sokal, Chromatic roots are dense in the whole complex plane, Combin. Probab. Comput. 13 (2004) 221–261, arXiv: cond-mat/0012369.
[30] A.D. Sokal, The multivariate Tutte polynomial (alias Potts model) for graphs and matroids, in: Bridget S. Webb (Ed.), Surveys in Combinatorics, 2005, Cambridge University Press, Cambridge, New York, 2005, pp. 173–226, arXiv:math.CO/0503607.
[31] A.D. Sokal, Real-variables characterization of generalized Stieltjes functions, Expo. Math. 28 (2010) 179–185, arXiv:0902.0065 [math.CA].
[32] R.P. Stanley, Enumerative Combinatorics, vol. 2, Cambridge University Press, Cambridge, New York, 1999.
[33] D.V. Widder, The Laplace Transform, Princeton University Press, Princeton, 1946.
[34] F.Y. Wu, The Potts model, Rev. Modern Phys. 54 (1982) 235–268; Erratum: Rev. Modern Phys. 55 (1983) 315.
[35] F.Y. Wu, Potts model of magnetism (invited), J. Appl. Phys. 55 (1984) 2421–2425.
[36] C.N. Yang, T.D. Lee, Statistical theory of equations of state and phase transitions, I. Theory of condensation, Phys. Rev. 87 (1952) 404–409.
[37] G.M. Ziegler, Lectures on Polytopes, Springer-Verlag, New York, 1995.